

Crystal Frameworks, Rigidity Operators and the RUM spectrum

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Bar-joint/bond-node frameworks. Rigidity matrix.

Crystal frameworks, Hilbert space operators, matrix functions

RUM spectrum = Low energy phonon spectrum.

The polynomial of a crystal.

Remarks on Symmetry - symmetrising Maxwell counting

Semi-infinite crystals and Toeplitz operators.

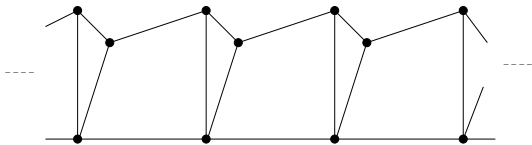


Figure: A \mathbb{Z} -periodic bar-joint framework.

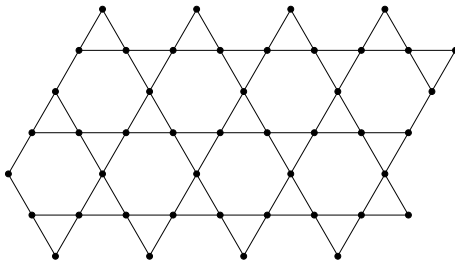


Figure: The **kagome** framework.

Questions :

Is the structure flexible ? rigid ?

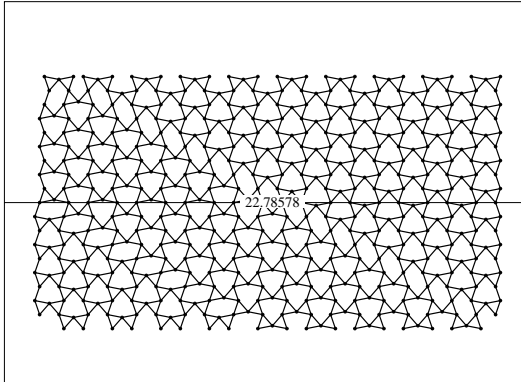
In what manner is it flexible ? rigid ?

How are the combinatorics of graphs implicated ?

How does symmetry affect rigidity ?

Two arenas: "deformations" and "infinitesimal flexes"

A "finite" deformation of the kagome framework:



Bar-joint frameworks - brief overview.

Watt, Peaucellier, Cauchy, Euler, Kempe, Maxwell, Laman.

THM Laman 1970:

N. and S. condition for a **generic** framework in 2D to be "just rigid":
Graph has Maxwell count $2V - E = 3$ together with the counting inequalities

$$2V' - E' \geq 3$$

for all sub-frameworks.

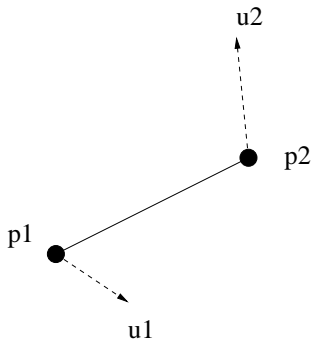


Figure: Infinitesimal flex velocities - no first order length change.

Notation for a crystal framework

Joints	Edges	Velocities
$p_{\kappa,k}$	$[p_{\kappa,k}, p_{\tau,l}]$	$u_{\kappa,k}$

Some classes of infinitesimal velocity vectors for (G, p) with $p = (p_i)$:

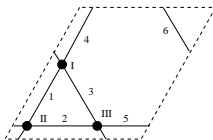
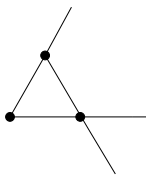
1. arbitrary : $u = (u_i), u_i \in \mathbb{R}^d$.
2. bounded : $|u_i| \leq K$ for all i .
3. vanishing : $|u_i| \rightarrow 0$ as $i \rightarrow \infty$.
4. square summable : $\sum_{i=1}^{\infty} |u_i|^2 < \infty$.
5. summable : $\sum_{i=1}^{\infty} |u_i| < \infty$.

DEF: (G, p) is **summably infinitesimally rigid** if there is no nonzero summable u with $R(G, p)u = 0$.

.. and so on.

A **crystal framework** \mathcal{C} is a bar-joint framework generated by a discrete translation group \mathcal{T} and a finite "motif".

eg. **Motif** (F_v, F_e) and **Unit Cell** :



DEF: A **crystal framework** \mathcal{C} is a triple (F_v, F_e, \mathcal{T})

An **infinitesimal flex** of \mathcal{C} : a vector of velocity vectors

$$u = (u_{\kappa,k}) \in \mathcal{H}_v = \prod_{\kappa,k} \mathbb{R}^d$$

such that for each edge $e = [p_{\kappa,k}, p_{\tau,l}]$

$$\langle p_{\kappa,k} - p_{\tau,l}, u_{\kappa,k} - u_{\tau,l} \rangle = 0.$$

Equivalently

$$R(G, p)u = 0$$

where the **rigidity matrix** whose e^{th} row is

$$[0 \dots 0 \quad v_e \quad 0 \dots 0 - v_e \quad 0 \dots 0]$$

where v_e is edge vector $p_{\kappa,k} - p_{\tau,l}$ appearing in columns for κ , and for τ (with sign $-$).

THM: (Owen-P, 2009)

The infinite rigidity matrix $R(G, p)$ for a crystal framework \mathcal{C} in \mathbb{R}^d determines a Hilbert space multiplication operator

$$M_\Phi : L^2(\mathbb{T}^d) \otimes \mathbb{C}^n \rightarrow L^2(\mathbb{T}^d) \otimes \mathbb{C}^m$$

whose symbol function $\Phi : \mathbb{T}^d \rightarrow M_{m,n}(\mathbb{C})$ is an $m \times n$ matrix-valued function on the d -torus determined by a motif.

DEF: $\Phi_{\mathcal{C}}$ is the **symbol function** of \mathcal{C} (with \mathcal{T}).
 $m = |F_e|$ rows, and $n = d|F_v|$ columns.

For the **kagome framework** \mathcal{C}_{kag} the symbol function $\Phi_{\text{kag}}(z, w)$ is

$$\frac{1}{4} \begin{bmatrix} -2 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 1 & -\sqrt{3} & -1 & \sqrt{3} \\ -1 & -\sqrt{3} & 0 & 0 & 1 & \sqrt{3} \\ 2 & 0 & -2z & 0 & 0 & 0 \\ 0 & 0 & -1 & \sqrt{3} & \bar{z}w & -\sqrt{3}\bar{z}w \\ \bar{w} & \sqrt{3}\bar{w} & 0 & 0 & -1 & -\sqrt{3} \end{bmatrix}$$

Also

$$\det \Phi_{\text{kag}}(z, w) = c\bar{z}w(z-1)(w-1)(z-w).$$

COR: The kagome framework is square-summably infinitesimally rigid (and hence summably infinitesimally rigid).

PROOF: $\Phi_{\text{kag}}(z, w)$ has full rank almost everywhere.

Some 3D frameworks:

The kagome net $\mathcal{C}_{\text{knet}}$

Sodalite \mathcal{C}_{SOD}

- a tetrahedral net

- a tetrahedral net

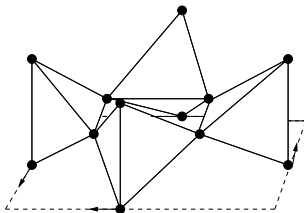


Figure: The top 4-ring of the sodalite cage.

Paulingite \mathcal{C}_{PAU}

Perovskite \mathcal{C}_{OCT}

- a tetrahedral net, with large unit cell

- simplest octahedron net

THM: The following are equivalent for a crystal framework \mathcal{C} :

- (i) There exists a nonzero square-summable infinitesimal flex.
- (ii) There exists a finitely supported ("local") infinitesimal flex.

This can be proven to hold for the frameworks for the zeolites [sodalite](#) and [paulingite](#) for example.

For sodalite $\Phi(z, w, u)$ is a 72×72 matrix.

Proof ... to input

The RUM spectrum $\Omega(\mathcal{C})$

More infinitesimal displacements u

For 2d frameworks with translation symmetries $x \rightarrow x + k, k \in \mathbb{Z}^2$:

1. periodic (= strict periodic = unit cell periodic):

$$u_{\kappa,i} = u_{\kappa,i+k}, \quad i, k \in \mathbb{Z}^2$$

2. supercell periodic:

$$u_{\kappa,i} = u_{\kappa,i+k}, \quad k \in n_1\mathbb{Z} \times n_2\mathbb{Z}. \quad \text{"floppy modes" context}$$

3. phase periodic : enlarge to complex scalar flexes:

$$u_{\kappa,i} = \omega^k u_{\kappa,i+k}, \quad i, k \in \mathbb{Z}^2 \quad \text{phase factor } \omega^k = \omega_1^{k_1} \omega_2^{k_2} \text{ with } (\omega_1, \omega_2) \in \mathbb{T}^2.$$

\mathcal{K}_v^ω : finite-dimensional vector space of phase-periodic velocity vectors.

THM. Let \mathcal{C} be a crystal framework with symbol $\Phi_{\mathcal{C}}(z)$. For ω in \mathbb{T}^d the restriction of $R(\mathcal{C}) : \mathcal{K}_v \rightarrow \mathcal{K}_e$ to the finite-dimensional space \mathcal{K}_v^ω has representing matrix $\Phi_{\mathcal{C}}(\bar{\omega})$.

Also

$u = (u_\kappa) \in \ker \Phi_{\mathcal{C}}(\bar{\omega})$ if and only if $\tilde{u} \in \ker R(\mathcal{C})$, where

$$\tilde{u}_{\kappa,k} = \omega^k u_\kappa,$$

Rigid Unit Mode spectrum of a crystal framework

DEF:

(i) The **RUM spectrum** of \mathcal{C} is the set $\Omega(\mathcal{C})$ of points $\omega = (\omega_1, \omega_2, \omega_3)$ in \mathbb{T}^3 with a nonzero ω -periodic flex:

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

(ii) The **RUM dimension** $\dim_{rum}(\mathcal{C})$ of \mathcal{C} is the dimension of the real algebraic variety $\Omega(\mathcal{C})$.

THM: The following are equivalent for a crystal framework \mathcal{C} :

(i) there is a square-summable infinitesimal flex.

(ii) there is a local infinitesimal flex.

(iii) \mathcal{C} has RUM dimension 3, or equivalently, $\Omega = \mathbb{T}^3$.

(iv) the supercell floppy modes have "order N " as $N \rightarrow \infty$:

(ie the order is equivalent to number of supercell atoms)

Wave vector formalism (phonons)

Phase $\omega = (\omega_1, \omega_2, \omega_3)$ in the 3-torus has wave vector $\mathbf{k} = (k_1, k_2, k_3)$ in $[0, 1)^3$, where $\omega_j = \exp(2\pi i k_j)$.

THM [P] The following are equivalent.

- (i) $(\omega^k u_\kappa)_{\kappa, k}$ is a nonzero infinitesimal **flex** for \mathcal{C} .
- (ii) For the **vertex wave motion**

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

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

$$|p_{\kappa, k}(t) - p_{\tau, l}(t)| - |p_{\kappa, k}(0) - p_{\tau, l}(0)|,$$

for the edges e **tend to zero** uniformly, in t and e , as the frequency α tends to zero.

Phase transition and RUM spectrum

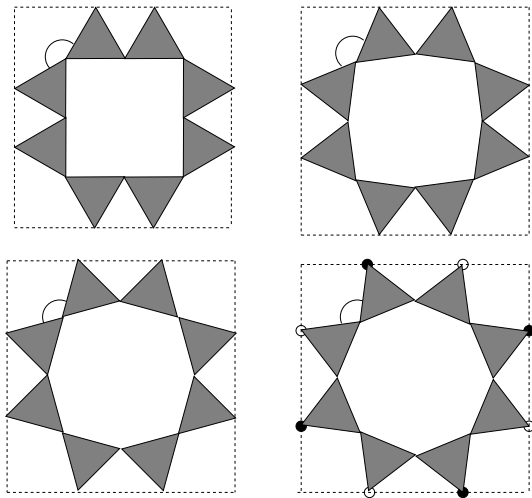


Figure: Unit cell deformations with angle $10\pi/12$, $9\pi/12$, $8\pi/12$, $7\pi/12$.

Exotic (non-linear) RUM spectrum.
 $\Omega(\mathcal{C})$ for the regular octagon framework:

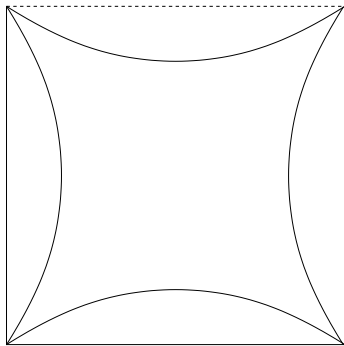


Figure: The curved wave vector spectrum of \mathcal{C}_{oct} .

Factoring the polynomial.

The octagon ring :

$$p_{\text{e}_{\text{oct}}}(z, w) = z^4 w^2 + z^2 w^4 - 2\sqrt{3}(z^3 w^3 + z^3 w + w^3 z + zw) + \\ (4\sqrt{3} - 4)(z^3 w^2 + z^2 w^3 - 2z^2 w^2 + z^2 w + zw^2) + w^2 + z^2$$

and factors as $p_1(z, w)p_2(z, w)$,

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

$$p_2(z, w) = z^2 w - (\sqrt{3} - \sqrt{2})zw^2 + 2(\sqrt{3} - \sqrt{2} - 1)zw - (\sqrt{3} - \sqrt{2})z + w.$$

For other exotic spectra see [Franz Wegner](#): Rigid-unit modes in tetrahedral crystals,

J. Phys.: Condens. Matter 2007

Capturing the Symmetry of \mathcal{C}

Let $\rho_{\text{sp}} : g \rightarrow T_g$ from space group $\mathcal{G}(\mathcal{C})$ to (affine) isometries of \mathbb{R}^d . Then for

$$R(\mathcal{C}) : \mathcal{H}_v \rightarrow \mathcal{H}_e,$$

$$\rho_e(g)R(\mathcal{C}) = R(\mathcal{C})\tilde{\rho}_v(g), \quad g \in \mathcal{G}(\mathcal{C}),$$

where

$$\tilde{\rho}_v = \rho_v \otimes \rho_{\text{sp}}$$

and where ρ_e and ρ_v are natural (linear) representations of $\mathcal{G}(\mathcal{C})$, associated with edges and with vertices.

whence operator methods, group representation methods, invariant subspaces, ...

Maxwell-Calladine counting formulae

For a 3D **finite** framework (G, p)

$$\text{"mechanism" dimension} - \text{selfstress dimension} = 3|V| - |E| - 6$$

[Fowler-Guest] Let σ be a spatial symmetry:

$$m_\sigma - s_\sigma = 3|V_\sigma| - |E_\sigma| - f_\sigma.$$

[P] **Crystal affine flex variant.** Let σ be an element of the point group of \mathcal{C} with space group representative g . Then

$$m_\sigma - s_\sigma = 3|F_v^\sigma| - |F_e^\sigma| + \dim \mathcal{E}_g - f_\sigma,$$

appropriately interpreted - m_σ = dimension of affinely-periodic mechanisms, periodic self-stresses ..

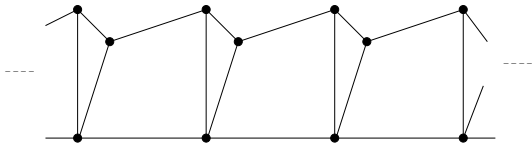


Figure: The \mathbb{Z} -periodic bar-joint framework also provides two semi-infinite frameworks.

Symbol function:

$$\Phi(z) = \begin{bmatrix} 0 & -4 & 0 & 4 & 0 & 0 \\ 0 & 0 & -1 & 1 & 1 & -1 \\ -1 & -3 & 0 & 0 & 1 & 3 \\ -4(1 - \bar{z}) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3\bar{z} & \bar{z} & -3 & -1 \end{bmatrix}.$$

Grounded framework matrix function:

$$\Phi_0(z) = \begin{bmatrix} 0 & 4 & 0 & 0 \\ -1 & 1 & 1 & -1 \\ 0 & 0 & 1 & 3 \\ 3\bar{z} & \bar{z} & -3 & -1 \end{bmatrix}.$$

$\det \Phi_0(z) = 16(2 - 3\bar{z})$: Only the right semi-infinite framework has a square-summable infinitesimal flex: T_{Φ_0} has kernel, whereas $T_{\Phi_0}^*$ does not.

Some ArXiv preprints

J.C. Owen and S.C. Power, Infinite bar-joint frameworks, SAC 2009.

J.C. Owen and S.C. Power, Frameworks, symmetry and rigidity, IJCGA

J.C. Owen and S.C. Power, Infinite Bar-Joint Frameworks, Crystals and Operator Theory, NYJM ..

A. Nixon, J.C. Owen and S.C. Power, Rigidity of frameworks supported on surfaces.

S.C. Power, Polynomials for crystal frameworks and the rigid unit mode spectrum.

S.C. Power, Crystal frameworks, symmetry and affinely periodic flexes.