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Generically globally rigid zeolites in the plane

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ABSTRACT

A d-dimensional zeolite is a d-dimensional body-and-pin framework with a $(d+1)$-regular underlying graph G. That is, each body of the zeolite is incident with $d+1$ pins and each pin belongs to exactly two bodies. The corresponding d-dimensional combinatorial zeolite is a bar-and-joint framework whose graph is the line graph of G.

We show that a two-dimensional combinatorial zeolite is generically globally rigid if and only if its underlying 3-regular graph G is 3-edge-connected. The proof is based on a new rank formula for the two-dimensional rigidity matroid of line graphs.

1. Introduction

A *d-dimensional zeolite* is a d-dimensional body-and-pin framework in which each body is incident with $d+1$ pins and each pin belongs to exactly two bodies. In the underlying graph G of the zeolite vertices correspond to bodies and two vertices are adjacent if and only if the corresponding bodies share a pin. Thus the underlying graph of the zeolite is $(d+1)$-regular.

By replacing the bodies by complete bar frameworks one obtains a *d-dimensional combinatorial zeolite*. It is a bar-and-joint framework whose graph is the line graph of the underlying graph G of the zeolite. (The *line graph* $L(G)$ of a graph $G=(V,E)$ is the simple graph with vertex set $\{v_e\colon e\in E\}$, where two vertices v_e, v_f are adjacent if and only if e, f have a common end-vertex in G.) See Fig. 1 for a two-dimensional example.

The investigation of these structures is motivated in part by the existence (and flexibility properties) of real zeolites, which are molecules formed by corner-sharing tetrahedra, see e.g. [3]. Planar plate frameworks (which contain planar zeolites as a special case), in which the bodies are pairwise congruent regular polygons, have also been studied in the rigidity literature [2]. The existence (or rigidity) of a unit distance realization of a given zeolite (or zeolites of a given size) without overlapping bodies is a related – and typically quite difficult – geometric question, see e.g. [4]. In this paper we shall consider the combinatorial aspects of zeolites and investigate (global) rigidity properties of planar combinatorial zeolites in generic position.

Roughly speaking, a combinatorial zeolite is globally rigid if its bar lengths uniquely determine the whole framework, up to congruence. Brigitte Servatius and Herman Servatius [11] asked whether there is a simple necessary and sufficient condition, in terms of its underlying graph, for the global rigidity of a planar zeolite whose vertices are in generic position. We shall give an affirmative answer in Section 3 by showing that a planar combinatorial zeolite is generically globally rigid if and only if its 3-regular underlying graph is 3-edge-connected. The proof is based on a new rank formula for the two-dimensional rigidity matroid of line graphs. This formula, along with the necessary definitions, is given in Section 2. The last section is devoted to some concluding remarks.

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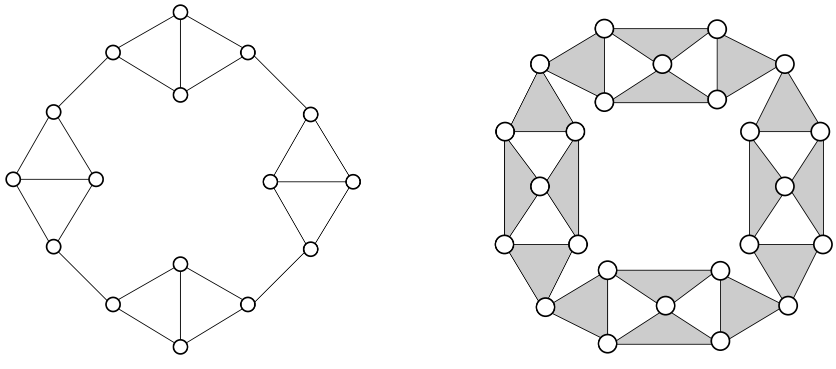

Fig. 1. A 3-regular graph G and its line graph $L(G)$. The shaded triangles of the bar-and-joint framework on $L(G)$ correspond to the bodies in the two-dimensional zeolite whose underlying graph is G.

2. Rigidity of line graphs

We shall need the following basic notions of combinatorial rigidity. For a detailed survey of the area we refer the reader to [1,12,13]. A d-dimensional (bar-and-joint) *framework* is a pair (G, p), where $G = (V, E)$ is a graph and p is a map from V to $\mathbb{R}^d$. We also say that (G, p) is a *realization* of G in $\mathbb{R}^d$. We can think of the edges and vertices of G in the framework as rigid (fixed length) bars and universal joints, respectively. Two frameworks (G, p) and (G, q) are *equivalent* if corresponding edges have the same lengths, that is, if $\|p(u) - p(v)\| = \|q(u) - q(v)\|$ holds for all pairs u, v with $uv \in E$, where $\|.\|$ denotes the Euclidean norm in $\mathbb{R}^d$. Frameworks (G, p), (G, q) are *congruent* if $\|p(u) - p(v)\| = \|q(u) - q(v)\|$ holds for all pairs u, v with $u, v \in V$. We shall say that (G, p) is *globally rigid* if every framework which is equivalent to (G, p) is congruent to (G, p).

Rigidity is a weaker property of frameworks than global rigidity. Intuitively, a framework is rigid if it has no continuous deformations. Equivalently, and more formally, a framework (G, p) is *rigid* if there exists an $\epsilon > 0$ such that, if (G, q) is equivalent to (G, p) and $\|p(u) - q(u)\| < \epsilon$ for all $v \in V$, then (G, q) is congruent to (G, p).

A framework (G, p) is said to be *generic* if the set containing the coordinates of all its points is algebraically independent over the rationals. It is known that rigidity as well as global rigidity are generic properties of d-dimensional frameworks for all d, that is, the (global) rigidity of a generic realization of a graph G depends only on the graph G and not the particular realization. We say that the graph G is *rigid*, respectively *globally rigid*, in $\mathbb{R}^d$ if every (or equivalently, if some) generic realization of G in $\mathbb{R}^d$ is rigid, respectively globally rigid. Many of the (global) rigidity properties of a generic framework (G, p) are determined by an associated matroid, the *d-dimensional rigidity matroid* $\mathcal{R}_d(G)$, defined on the edge set of G. We denote the rank of $\mathcal{R}_d(G)$ by $r_d(G)$.

In what follows we shall focus on the case $d = 2$. In this case rigidity and the rank function of the rigidity matroid are well characterized. It is known that a graph $G = (V, E)$ is rigid in $\mathbb{R}^2$ if and only if $r_2(G) = 2|V| - 3$. It is also known that the edge set of G is independent in $\mathcal{R}_2(G)$ if and only if each subset $X \subseteq V$ with $|X| \geqslant 2$ induces at most $2|X| - 3$ edges [8]. Lovász and Yemini [9] characterized rigid graphs in $\mathbb{R}^2$ by providing a formula for $r_2(G)$, in terms of 'thin covers' of G. We shall use the following refinement of their result, which uses rigid components, see [1, Section 4.4]. We define a *rigid component* of a graph $G = (V, E)$ to be a maximal rigid subgraph of G. By the *glueing lemma* (see [12, Lemma 3.1.4]), which says that the union of two rigid graphs with at least two vertices in common is rigid, it follows that any two rigid components of G intersect in at most one vertex. Thus their vertex sets form a special 'thin cover' of G.

Theorem 2.1. *(See [1,9].) Let $H = (V, E)$ be a graph with rigid components $H_1, H_2, \ldots, H_t$. Then*

$$r_2(H) = \sum_{i=1}^{t} \bigl(2|C_i| - 3\bigr),$$

where $C_i = V(H_i)$, $1 \leqslant i \leqslant t$.

Let $G = (V, E)$ be a graph. For a family $\mathcal{F}$ of pairwise disjoint subsets of V let $E_G(\mathcal{F})$ denote the set, and $e_G(\mathcal{F})$ the number, of edges of G connecting distinct members of $\mathcal{F}$. For a partition $\mathcal{P}$ of V let

$$\mathrm{def}_G(\mathcal{P}) = 3\bigl(|\mathcal{P}| - 1\bigr) - 2e_G(\mathcal{P})$$

denote the *deficiency* of $\mathcal{P}$ in G and let

$$\mathrm{def}(G) = \max\bigl\{\mathrm{def}_G(\mathcal{P}):\ \mathcal{P} \text{ is a partition of } V\bigr\}.$$

We say that a partition $\mathcal{P}$ of V is *tight* if $\mathrm{def}_G(\mathcal{P}) = \mathrm{def}(G)$ holds. Note that $\mathrm{def}(G) \geqslant 0$, since $\mathrm{def}_G(\{V\}) = 0$. For example, the graph G in Fig. 1 has $\mathrm{def}(G) = 1$. The vertex sets of the four disjoint copies of 'K_4 minus an edge' in G form a tight partition of G.

The following rank formula (which is implicit in [7]) shows that the 'degree of freedom' of $L(G)$ is equal to the deficiency of G.

Theorem 2.2. *Let $G = (V, E)$ be a graph with minimum degree at least two. Then*

$$r_2\bigl(L(G)\bigr) = 2|E| - 3 - \mathrm{def}(G). \tag{1}$$