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Rigid components in molecular graphs

Bill Jackson and Tibor Jordán

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Bill Jackson* and Tibor Jordán**

Abstract

In this paper we consider 3-dimensional generic bar-and-joint realizations of squares of graphs. These graphs are also called molecular graphs due to their importance in the study of flexibility in molecules. The Molecular Conjecture, posed in 1984 by T-S. Tay and W. Whiteley, indicates that determining rigidity (or more generally, computing the degree of freedom) of squares of graphs may be tractable by combinatorial methods. We show that the truth of the Molecular Conjecture would imply an efficient algorithm to identify the maximal rigid subgraphs of a molecular graph. In addition, we prove that the truth of two other conjectures in combinatorial rigidity (due to A. Dress and D. Jacobs, respectively) would imply the truth of the Molecular Conjecture.

1 Introduction

All graphs considered are finite and without loops. We will reserve the term graph for graphs without multiple edges and refer to graphs which may contain multiple edges as *multigraphs*. Let $\mathcal{R}(G)$ denote the 3-dimensional *generic bar-and-joint rigidity matroid* of G, defined on ground-set E. (See [8, 18] for the definition of $\mathcal{R}(G)$.) We denote the rank function of $\mathcal{R}(G)$ by r_G and $r_G(E)$ by $r(G)$. By a result of Gluck [5] a graph $G = (V, E)$ on at least three vertices has $r(G) \leq 3|V| - 6$. A graph $G = (V, E)$ is said to be *rigid* if either G is a complete graph on at most two vertices, or $|V| \geq 3$ and $r(G) = 3|V| - 6$. It is a difficult open problem to determine which graphs are rigid. For a survey and partial results see [3, 6, 7, 8, 9, 18].

The *square* of a graph $G = (V, E)$ is denoted by G^2, and the multigraph obtained from G by replacing each edge $e \in E$ by five copies of e is denoted by $5G$. Squares of graphs are sometimes called *molecular graphs*, because they are used to study the flexibility of molecules, particularly biomolecules such as proteins [12, 17, 22]. The Molecular Conjecture, due to Tay and Whiteley [16, Conjecture 1], see also [13, 18, 19, 20, 21, 22], indicates that the problem of determining when molecular

*School of Mathematical Sciences, Queen Mary, University of London, Mile End Road, London E1 4NS, England. e-mail: b.jackson@qmul.ac.uk

**Department of Operations Research, Eötvös University, Pázmány Péter sétány 1/C, 1117 Budapest, Hungary. e-mail: jordan@cs.elte.hu. Supported by the MTA-ELTE Egerváry Research Group on Combinatorial Optimization and the Hungarian Scientific Research Fund grant no. T049671.

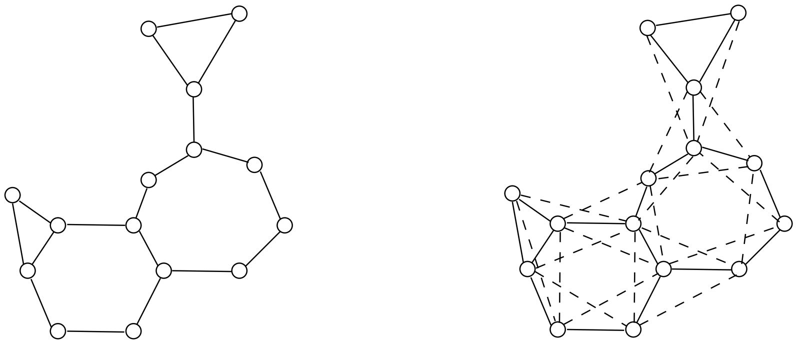

Figure 1: A graph G and its square G^2.

graphs are rigid (or more generally, finding their maximal rigid subgraphs) may be significantly easier than the problem for arbitrary graphs. For a substantial collection of supporting evidence for the Molecular Conjecture see [22].

This conjecture appears in the literature in several different forms, and is typically formulated in terms of 'body-and-hinge frameworks'. In this paper we shall be concerned with bar-and-joint frameworks. Conjectures 1.1 and 1.2 below are the bar-and-joint versions of the Molecular Conjecture.

Conjecture 1.1. *Let G be a graph with minimum degree at least two. Then G^2 is rigid if and only if $5G$ contains six edge-disjoint spanning trees.*

The 'defect form' of Conjecture 1.1 is the following. 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

$$\mathrm{def}_G(\mathcal{P}) = 6(|\mathcal{P}| - 1) - 5e_G(\mathcal{P})$$

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

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

Note that $\mathrm{def}(G) \geq 0$ since $\mathrm{def}_G(\{V\}) = 0$.

Conjecture 1.2. *[10] Let $G = (V, E)$ be a graph with minimum degree at least two. Then*

$$r(G^2) = 3|V| - 6 - \mathit{def}(G). \tag{1}$$

We showed in an earlier paper [10] that Conjectures 1.1 and 1.2 are equivalent. We also showed that the right hand side of (1) is an upper bound on the rank of G^2.

Theorem 1.3. *[10] Let $G = (V, E)$ be a graph of minimum degree at least two. Then*

$$r(G^2) \leq 3|V| - 6 - \mathit{def}(G).$$

In this paper we shall prove a number of structural properties of maximal rigid subgraphs of a molecular graph. Based on these results, we show that the truth of the Molecular Conjecture would imply an efficient algorithm which can identify these subgraphs by finding the maximal subgraphs of $5G$ which contain six edge-disjoint spanning trees. Jacobs [11] gives a different algorithm for finding the maximal rigid subgraphs of a molecular graph (see also [12]), but there is no rigorous proof for the correctness of his algorithm even if we assume that the Molecular Conjecture is true.

In addition, we prove that the truth of two other conjectures in combinatorial rigidity (due to Dress and Jacobs, respectively) would imply the truth of the Molecular Conjecture.

2 Preliminaries

Let $G = (V, E)$ be a multigraph. For $X \subseteq V$, let $E_G(X)$ denote the set, and $i_G(X)$ the number, of edges in $G[X]$, that is, in the subgraph induced by X in G. For $X \subset V$ let $d_G(X) = e_G(X, V - X)$ denote the *degree* of X. If $X = \{v\}$ for some $v \in V$ then we simply write $d_G(v)$ for the degree of v. The set of *neighbours* of X (i.e. the set of those vertices $v \in V - X$ for which there exists an edge $uv \in E$ with $u \in X$) is denoted by $N_G(X)$. We use $E(X)$, $i(X)$, $d(X)$, or $N(X)$ when the multigraph G is clear from the context. A graph $G = (V, E)$ is *M-independent*, or an *M-circuit* if E is independent, respectively a circuit, in $\mathcal{R}(G)$.

We shall use the following concepts and basic results from graph (rigidity) theory.

Lemma 2.1. *[18, Lemma 9.1.3] Let $H = (V, E)$ be a graph and $v_1, v_2, \ldots v_s$ be distinct vertices of G for some $s \in \{1, 2, 3\}$. Let G be obtained from H by adding a new vertex v and all edges vv_i for $1 \le i \le s$. Then G is M-independent if and only if H is M-independent.*

Lemma 2.2. *[18, Lemma 9.2.2] Let $H = (V, E)$ be an M-independent graph and $v_i \in V$ be distinct vertices for $1 \le i \le 4$. Suppose $v_1v_2 \in E$. Let G be obtained from $H - v_1v_2$ by adding a new vertex v and all edges vv_i for $1 \le i \le 4$. Then G is M-independent.*

We refer to the operations in Lemmas 2.1 and 2.2 as 0-*extensions* and 1-*extensions*, respectively.

Lemma 2.3. *[10] Let $H = (V, E)$ be an M-independent graph and $\{u_1, u_2\}$, $\{v_1, v_2\}$ and $\{w_1, w_2\}$ be three sets of distinct vertices of G with $|\{u_1, u_2, v_1, v_2, w_1, w_2\}| \ge 3$. Let G be obtained from H by adding three new vertices u, v, w, the edges uv, vw, uw, and all edges uu_i, vv_i, ww_i for $1 \le i \le 2$. Then G is M-independent.*

We refer to the operation in Lemma 2.3 as a *triangle-extension*.

Lemma 2.4. *[18, Lemma 11.1.9] (a) If $|V(G_1) \cap V(G_2)| \ge 3$ and G_1, G_2 are rigid then $G_1 \cup G_2$ is rigid.*
(b) If G is rigid and has at least four vertices then G is 3-connected.

Lemma 2.5. *Let G_1, G_2 be rigid graphs with $|V(G_1) \cap V(G_2)| = 2$. Let $H = G_1 \cup G_2 \cup \{uv\}$ for some $u \in V(G_1) - V(G_2)$ and $v \in V(G_2) - V(G_1)$. Then H is rigid.*

Proof: We may suppose that G_1, G_2 are minimally rigid. Let $V(G_1 \cap G_2) = \{x_1, x_2\}$. The rigidity of G_2 implies that vx_i is contained in an M-circuit C_i in $G_2 + vx_i$, for $i \in \{1, 2\}$. Let $H_1 = G_1 + v + \{vu, vx_1, vx_2\}$ and $H_2 = G_2 + \{vx_1, vx_2\}$. The rigidity of G_1, G_2 and Lemma 2.1 imply that H_1 and H_2 are both rigid. Thus $H_1 \cup H_2$ is rigid by Lemma 2.4(a). The existence of the M-circuits C_1, C_2 implies that $H = (H_1 \cup H_2) - \{vx_1, vx_2\}$ is also rigid. •

A *cover* of a graph $G = (V, E)$ is a collection $\mathcal{X}$ of subsets of V, each of size at least two, such that $\cup_{X \in \mathcal{X}} E(X) = E$. A cover $\mathcal{X} = \{X_1, X_2, \dots, X_m\}$ of G is *t-thin* if $|X_i \cap X_j| \leq t$ for all $1 \leq i < j \leq m$. For $X_i \in \mathcal{X}$ let $f(X_i) = 1$ if $|X_i| = 2$ and $f(X_i) = 3|X_i| - 6$ if $|X_i| \geq 3$. Given a 2-thin cover $\mathcal{X}$ of G, let $\Theta(\mathcal{X})$ be the set of all pairs of vertices uv such that $X_i \cap X_j = \{u, v\}$ for some $1 \leq i < j \leq m$. For each $uv \in \Theta(\mathcal{X})$ let $\theta(uv)$ be the number of sets X_i in $\mathcal{X}$ such that $\{u, v\} \subseteq X_i$ and put

$$val(\mathcal{X}) = \sum_{X \in \mathcal{X}} f(X) - \sum_{uv \in \Theta(\mathcal{X})} (\theta(uv) - 1). \tag{2}$$

For $u, v \in V$, the edge uv is an *implied edge* of G if $uv \notin E$ and $r(E + uv) = r(E)$. The closure $\hat{G}$ of G is the graph obtained by adding all the implied edges to G. A *rigid cluster* of G is a set of vertices which induce a maximal complete subgraph of $\hat{G}$. Using Lemma 2.4(a), we can see that any two rigid clusters of G intersect in at most two vertices. Thus the set of rigid clusters of G is a 2-thin cover of G. At a conference on rigidity held in Montreal in 1987, Dress conjectured that the value of this special 2-thin cover is equal to the rank of G.

Conjecture 2.6. *(see [6, Conjecture 5.6.1],[2], and [15, Conjecture 2.3]) Let $G = (V, E)$ be a graph and $\mathcal{X}$ be the set of rigid clusters of G. Then*

$$r(G) = val(\mathcal{X}). \tag{3}$$

We say that a cover $\mathcal{X}$ of a graph $G = (V, E)$ is *independent* if the graph $(V, \Theta(\mathcal{X}))$ is M-independent. The following lemma shows that independent covers of G can be used to give an upper bound on $r(G)$.

Lemma 2.7. *[8, Lemma 3.2] Let $G = (V, E)$ be a graph, and $\mathcal{X}$ be an independent 2-thin cover of G. Then $r(G) \leq val(\mathcal{X})$.*

Remark The proof given for Lemma 2.7 in [8] shows that it remains true under the weaker hypothesis that the subgraph of $(V, \Theta(\mathcal{X}))$ induced by X is M-independent for all $X \in \mathcal{X}$.

3 Rigid components of molecular graphs

We call the inclusionwise maximal rigid subgraphs of a graph H, the *rigid components* of H. Each rigid component is clearly an induced subgraph of H.

We first verify a number of properties of the rigid components of a molecular graph. We assume throughout this section that $G = (V, E)$ is a connected graph with $|V| \geq 3$ and with minimum degree at least two, and G^2 is its square. We refer to the edges in $E(G^2) - E(G)$ as *new edges* of G^2.

Lemma 3.1. *Let C be a rigid component of G^2 and let $Y = V(C)$. Then*
(a) $|Y| \geq 3$,
(b) $d_{G[Y]}(v) \geq 1$ for all $v \in Y$,
(c) $G[Y]$ is connected,
(d) $d_{G[Y]}(v) = 1$ for all $v \in N_G(V - Y)$.

Proof: (a) This follows from the fact that each edge of G^2 belongs to a triangle and hence to a rigid subgraph with three vertices.

(b) Suppose that all the edges incident to v in $G^2[Y]$ are new edges. The new edges of G^2 are 'generated' by pairs of edges of G, and, by our assumption, these edges cannot be in $G[Y]$. First suppose $|Y| \geq 4$. Then we have (at least) three new edges e, f, g incident to v in $G^2[Y]$. By considering the pairs of edges of G which 'generate' e, f, g, and the edges that these pairs 'generate' in $V - Y$, it is easy to check that either there is a vertex $y \in V - Y$ connected to Y by three edges in G^2, or there is a triangle T in $G^2 - Y$ which satisfies the hypotheses of Lemma 2.3 in G^2. This contradicts the maximality of C by Lemma 2.1 or Lemma 2.3. Next suppose $|Y| = 3$. The proof of this case is similar by considering the two new edges e, f incident to v in G^2 as well as the third edge g of $G^2[Y]$.

(c) Consider a connected component D of $G[Y]$. By (b) each vertex of D is incident to an edge in $G[Y]$. Let uv, vw be a pair of edges in E which 'generate' a new edge uw connecting D and $G[Y] - D$. We must have $v \in V - Y$ and we can easily see that v must be connected to Y by at least three edges in G^2. This contradicts the maximality of C by Lemma 2.1.

(d) Let $uv \in E$ with $v \in Y$ and $u \in V - Y$. We have $d_{G[Y]}(v) \geq 1$ by (b). If $d_{G[Y]}(v) \geq 2$ then u must be connected to Y by at least three edges in G^2, a contradiction by Lemma 2.1 and the maximality of C. Thus $d_{G[Y]}(v) = 1$. •

Lemma 3.2. *Suppose that G^2 is not rigid. Let C_1, C_2 be distinct rigid components of G^2 with $Y_1 = V(C_1)$, $Y_2 = V(C_2)$ and $Y_1 \cap Y_2 = \{u, v\}$. Then*
(a) $uv \in E$,
(b) $d_{G[Y_1]}(u) = 1$ and $d_{G[Y_2]}(v) = 1$ (or $d_{G[Y_2]}(u) = 1$ and $d_{G[Y_1]}(v) = 1$),
(c) uv is contained in no rigid components of G other than C_1, C_2.

Proof: The maximality of C_1, C_2 implies that $Y_1 - Y_2 \neq \emptyset \neq Y_2 - Y_1$. Part (a) follows from Lemma 3.1(b), Lemma 2.5, and the maximality of C. Part (b) follows in a similar way from Lemma 2.5. Part (c) follows from (b) and Lemma 3.1(a),(c). •

Lemma 3.3. *Suppose that G^2 is not rigid. Let C_1, C_2 be distinct rigid components of G^2 with $Y_1 = V(C_1)$, $Y_2 = V(C_2)$ and $Y_1 \cap Y_2 = \{v\}$. Then $d_{G[Y_1]}(v) = 1 = d_{G[Y_2]}(v)$.*

Proof: The lemma follows from Lemma 3.1(b), Lemma 2.1, and the maximality of C. •

It follows from the fact that every edge is contained in a rigid component, and Lemma 2.4(a), that the vertex sets of the rigid components of a graph H form a 2-thin cover of H. We will abuse our notation and use $val(\mathcal{C})$ to denote the value of this 2-thin cover.

Lemma 3.4. *Suppose that G^2 is not rigid. Let $\mathcal{C} = \{C_1, C_2, \ldots, C_t\}$ be the set of rigid components of G^2. For all $1 \leq i \leq t$, let $Y_i = V(C_i)$ and let $Q_i = Y_i - \{v : d_{G[Y_i]} = 1\}$. Put $\mathcal{Q} = \{Q_1, Q_2, ..., Q_t\}$. Then*
(a) $\mathcal{Q}$ is a partition of V,
(b) $val(\mathcal{C}) = 3|V| - 6 - def_G(\mathcal{Q})$,
(c) $r(G^2) \leq val(\mathcal{C})$.

Proof: (a) By Lemma 3.1(a), (c), $Q_i \neq \emptyset$ for all $1 \leq i \leq t$. Choose $v \in V$. Since $d_G(v) \geq 2$, v is contained in a triangle in G^2 and hence in at least one member of $\mathcal{Q}$. On the other hand, Lemmas 3.2(b) and 3.3 imply that v does not belong to two different members of $\mathcal{Q}$. Thus $\mathcal{Q}$ partitions V.

(b) By Lemma 3.1(a) we have $|Y_i| \geq 3$ for all $1 \leq i \leq t$. By Lemma 3.2(a),(c) we have $uv \in E$ and $\theta(uv) = 2$ for all $uv \in \Theta(\mathcal{C})$. By Lemma 3.2(b) and the definition of $\mathcal{Q}$ we have $E_G(\mathcal{Q}) = \Theta(\mathcal{C})$. Lemma 2.1 implies that $N_G(Q_i) \subseteq Y_i$ and hence $|Y_i| = |Q_i| + d_G(Q_i)$ for all $1 \leq i \leq t$. Thus $val(\mathcal{C}) = \sum_{C_i \in \mathcal{C}}(3|Y_i| - 6) - |\Theta(\mathcal{C})| = 3|V| + 6e_G(\mathcal{Q}) - 6t - e_G(\mathcal{Q}) = 3|V| - 6 - \mathrm{def}_G(\mathcal{Q})$.

(c) Theorem 1.3 and (b) now imply

$$r(G^2) \leq 3|V| - 6 - \mathrm{def}(G) \leq 3|V| - 6 - \mathrm{def}_G(\mathcal{Q}) = val(\mathcal{C}).$$

•

We will refer to the partition $\mathcal{Q}$ defined in Lemma 3.4 as the *partition of V generated by the rigid components of G^2*.

Remark: Let H_i be the subgraph of $(V, \Theta(\mathcal{C}))$ induced by $V(C_i)$ for all $C_i \in \mathcal{C}$. Then each H_i is a forest by Lemma 3.2(b) and hence is M-independent. Thus $r(G^2) \leq val(\mathcal{C})$ also follows from the stronger version of Lemma 2.7 described in the remark after the statement of Lemma 2.7.

We conjecture that equality holds in Lemma 3.4(c).

Conjecture 3.5. *Let G be a graph of minimum degree at least two. Then $r(G^2) = val(\mathcal{C})$.*

We will show in the next section that this conjecture is equivalent to Conjecture 1.2.

Note that there exist examples of a graph H whose set of rigid components $\mathcal{C}$ satisfies $r(H) < val(\mathcal{C})$.[1] It is conceivable, however, that $r(H) \leq val(\mathcal{C})$ holds for all graphs H.

[1]Let $G_0 = (V_0, E_0)$ be a complete graph on five vertices with $V_0 = \{v_i : 1 \leq i \leq 5\}$. For

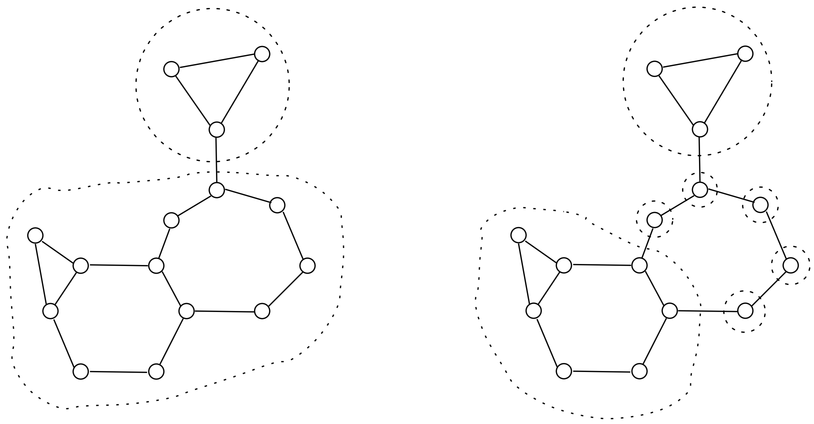

Figure 2: The brick partition and the superbrick partition of graph G.

4 Bricks and rigid components

Let $G = (V, E)$ be a graph of minimum degree two. In this section, we consider the relationship between the partition $\mathcal{Q}$ of V generated by the rigid components of G^2 and another partition of V. We say that the graph G is *strong* if $5G$ has six edge-disjoint spanning trees. A subgraph H is a *brick* of G if H is a maximal strong subgraph of G. Thus bricks are induced subgraphs of G. It was shown in [10] that the vertex sets of the bricks of $G = (V, E)$ partition V. We shall refer to this partition of V as the *brick partition* of G. We illustrate the brick partition of a graph in Figure 2. (We also give the 'superbrick partition', which is a refinement of the brick partition defined at the end of this section.) We showed in [10] that the brick partition $\mathcal{B}$ of G satisfies $\mathrm{def}_G(\mathcal{B}) = \mathrm{def}(G)$. We shall prove that $\mathcal{Q}$ is a refinement of $\mathcal{B}$, and that, if Conjecture 1.1 is true, then $\mathcal{Q} = \mathcal{B}$.

Let $L(H)$ denote the vertices of degree one in graph H.

Lemma 4.1. *Let G be a graph, C be a rigid component of G^2, $Y = V(C)$ and $X = Y - L(G[Y])$. Then $G[X]^2$ is rigid and $G[X]$ is strong.*

Proof: Since C is a rigid component of G^2, it follows from Lemma 2.1, Lemma 3.1 (a),(c), and the maximality of C that $|Y| \geq 3$, $G[Y]$ is connected, and $G^2[Y] = G[Y]^2$. Since $Y - X = L(G[Y])$, we also have $G[X]$ is connected and $G^2[X] = G[X]^2$. Furthermore, either $|X| = 1$, or $|X| \geq 3$ and $d_{G[X]}(v) \geq 2$ for all $v \in X$ (since the end-vertices of a cut-edge in $G[X]$ would form a separating pair in C, and, by Lemma 2.4(b), this would contradict the fact that C is rigid). If $|X| = 1$ then $G[X]^2$ is rigid and $G[X]$ is strong by definition. Hence we may suppose that $|X| \geq 3$.

Consider a set of vertices $W \subseteq Y - X$ whose unique neighbour in $G[Y]$ is the same vertex v. Then $v \in X$ and $d_{G[X]}(v) \geq 2$, so $G^2[\{v\} \cup N_{G[X]}(v)]$ is a complete graph

$1 \leq i < j \leq 5$ let $G_{i,j} = (V_{i,j}, E_{i,j})$ be a complete graph on five vertices with $V_{i,j} \cap V_0 = \{v_i, v_j\}$ and $E_{i,j} \cap E_0 = \{v_i v_j\}$ for $1 \leq i < j \leq 5$. Let $G = \left(G_0 \cup (\bigcup_{1 \leq i < j \leq 5} G_{i,j})\right) - E_0$. It can be seen that $r(G) \leq |E(G)| - 1 = 89$. On the other hand, the set of rigid components of G is $\mathcal{C} = \{V_{i,j} : 1 \leq i < j \leq 5\}$ and we have $val(\mathcal{C}) = 90$. See [9, Example 3] for more details.

K^v on at least three vertices. Thus we may choose a basis B^v for $\mathcal{R}(K^v)$, and hence a basis B for $\mathcal{R}(C)$, in which each vertex $w \in W$ has degree exactly three and there are no edges between vertices in W. Since C is rigid, Lemma 2.1 now implies that $C - W$ is also rigid. This argument may be repeated for each group of vertices $W' \subseteq Y - X$ with a common neighbour to deduce that $G[X]^2 = G^2[X] = C - (Y - X)$ is rigid. Theorem 1.3 now implies that $G[X]$ is strong. •

We showed in [10] that if two strong subgraphs have a non-empty intersection, then their union is strong. Together with Lemma 4.1, this implies that, for a graph $G = (V, E)$ of minimum degree at least two, the partition of V generated by the rigid components of G^2 is a refinement of the brick partition of G.

Lemma 4.2. *Let G be a graph, $B = G[X]$ be a strong subgraph of G and $Y = X \cup N_G(X)$. Suppose that Conjecture 1.1 holds for B. Then $G[Y]^2$ is rigid.*

Proof: If $|X| = 1$ then $G[Y]^2$ is a complete graph, and hence is rigid. Suppose $|X| \geq 3$. Since B is strong, B has minimum degree at least two. By Conjecture 1.1, $G[X]^2$ is rigid. Thus $G[Y]^2$ is rigid by Lemma 2.1. •

Lemma 4.3. *Let G be a graph of minimum degree at least two.*
(a) Let $B = G[X]$ be a brick of G, $Y = X \cup N_G(X)$, and suppose that Conjecture 1.1 holds for B. Then $G[Y]^2$ is a rigid component of G^2.
(b) Let C be a rigid component of G^2, $Y = V(C)$, and $X = Y - L(G[Y])$. Let B be the brick of G which contains $G[X]$ and suppose that Conjecture 1.1 holds for B. Then $B = G[X]$.

Proof: (a) Since $G[X]$ is a brick, each vertex in X has degree at least two in $G[Y]$ (if X is non-trivial, each vertex has degree at least two already in $G[X]$; if X is trivial, it follows from the fact that G has minimum degree at least two). By Lemma 4.2, $G[Y]^2$ is rigid. Let C be the rigid component of G^2 containing $G[Y]^2$ and let $Y' = V(C)$. Suppose $Y' - Y \neq \emptyset$. By Lemma 4.1, $X' = Y' - L(G[Y'])$ is strong. Now $X \subseteq X'$ since $X \cap L(G[Y']) = \emptyset$. Since X is a brick, we must have $X = X'$ and hence $Y = Y'$. Thus $G^2[Y]$ is a rigid component of G^2. Since B is a brick, it is easy to see that $G^2[Y] = G[Y]^2$.

(b) Since C is a rigid component of G^2, Lemma 4.1 implies that $G[X]$ is strong. Let $X' = V(B)$. By Lemma 4.2, $G[X' \cup N_G(X')]^2$ is rigid. Since C is a rigid component of G^2, we have $|Y| \geq 3$ by Lemma 3.1(a). Since $Y \subseteq X' \cup N_G(X')$ and C is a rigid component, we have $X' \cup N_G(X') = Y$. Thus $X' \subseteq Y$. But $d_{G[Y]}(v) = 1$ for all $v \in Y - X$, since $Y - X = L(G[Y])$. Since $X' \subseteq Y$ and $G[X']$ is a brick, we must have $v \notin X'$ for all $v \in Y - X$. Thus $X' = X$ and $B = G[X]$. •

By Lemmas 4.2 and 4.3 we obtain:

Corollary 4.4. *Suppose that Conjecture 1.1 holds. Let $G = (V, E)$ be a graph of minimum degree at least two. Then for each rigid component C of G^2 there is a brick $B = G[X]$ of G with $C = G[X \cup N_G(X)]^2$, and for each brick $B = G[X]$ of G the subgraph $G[X \cup N_G(X)]^2$ is a rigid component of G^2.*

Corollary 4.4 immediately implies that if Conjecture 1.1 holds then the partition $\mathcal{Q}$ of V generated by the rigid components of G^2 is identical to the brick partition $\mathcal{B}$ of G. We may now deduce:

Corollary 4.5. *Conjectures 1.1, 1.2 and 3.5 are all equivalent.*

Proof: The fact that Conjectures 1.1 and 1.2 are equivalent follows from [10]. We show that Conjectures 1.2 and 3.5 are equivalent. Let $G = (V, E)$ be a graph of minimum degree at least two. Let $\mathcal{B}$ be the brick partition of G, $\mathcal{C}$ be the set of rigid components of G^2, and $\mathcal{Q}$ be the partition of V generated by $\mathcal{C}$.

Suppose Conjecture 1.2 holds. Then $r(G^2) = 3|V| - 6 - \mathrm{def}(G)$. Since $\mathrm{def}_G(\mathcal{B}) = \mathrm{def}(G)$ by [10], $\mathcal{B} = \mathcal{Q}$ by the above, and $3|V| - 6 - \mathrm{def}_G(\mathcal{Q}) = val(\mathcal{C})$ by Lemma 3.4(b), we have $r(G^2) = val(\mathcal{C})$. Thus Conjecture 3.5 holds for G.

Suppose, on the other hand, that Conjecture 3.5 holds. Then

$$r(G^2) = val(\mathcal{C}) = 3|V| - 6 - \mathrm{def}_G(\mathcal{Q}) \geq 3|V| - 6 - \mathrm{def}(G) \geq r(G^2),$$

by Lemma 3.4(b), and Theorem 1.3. Thus equality holds throughout and Conjecture 1.2 holds for G. •

It was shown in [10] that, if true, Conjecture 1.2 could be used to determine the rank of squares of all graphs, not just graphs of minimum degree at least two. It is also possible to extend the results of Sections 3 and 4 to squares of arbitrary graphs. We omit the details.

A graph H is called *redundantly rigid* if $H - e$ is rigid for all $e \in E(H)$. In applications it is sometimes useful to identify the *redundantly rigid components* (that is, the maximal redundantly rigid subgraphs) of a molecular graph, see [12].

It would be interesting to find (possibly assuming the truth of Conjecture 1.1) a connection between the redundantly rigid components of G^2 and the 'superbrick partition' of G. We say that G is *superstrong* if $5G - e$ has six edge-disjoint spanning trees for all $e \in E(5G)$. A subgraph H of G is said to be a *superbrick* of G if H is a maximal superstrong subgraph of G. It was shown in [10] that the vertex sets of the superbricks of a graph $G = (V, E)$ partition V. We shall refer to this partition of V as the *superbrick partition* of G, see Figure 2.

As a first step, one may ask whether the square of a superstrong graph is redundantly rigid. This is not the case in general: consider, for example, the graph G_0 consisting of two 4-cycles joined at a cut-vertex. Then G_0 is superstrong but G_0^2 is not redundantly rigid since it contains vertices of degree three. It is conceivable, however, that if G is superstrong and G^2 has minimum degree at least four then G^2 is redundantly rigid.

5 Rigid clusters

A (3-dimensional) *framework* (G, p) is a graph $G = (V, E)$ together with a map $p : V \to \mathbb{R}^3$. We say that (G, p) is a *generic realization* of G if the set of coordinates

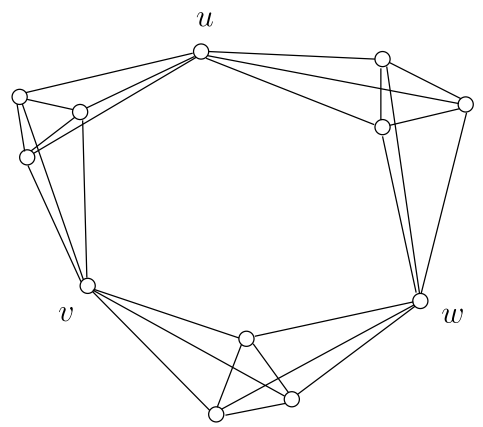

Figure 3: A graph H with a rigid cluster $U = \{u, v, w\}$ for which $H[U]$ is not rigid.

of all points $p(v)$, $v \in V$, is algebraically independent over $\mathbb{Q}$. A subset $U \subseteq V$ is a *rigid cluster* of (G, p) if U is a maximal subset of V with the property that there exists an $\epsilon > 0$ such that, for all frameworks (G, q) with $\|p(v) - q(v)\| < \epsilon$ for all $v \in V$ and $\|p(v) - p(w)\| = \|q(v) - q(w)\|$ for all $vw \in E$, we have $\|p(u) - p(u')\| = \|q(u) - q(u')\|$ for all $u, u' \in U$. (This is equivalent to saying that U is a maximal subset of V with the property that every 'continuous deformation' of (G, p) which preserves the lengths $\|p(v) - p(w)\|$ of all edges $vw \in E$, also preserves the distances $\|p(u) - p(u')\|$ between the points $p(u), p(u')$ for all $u, u' \in U$.) It is known that the rigid clusters of (G, p) are the same for all generic realizations of G, and correspond to the subsets of V defined as rigid clusters of G in Section 2. Thus we need to determine the rigid clusters of G in order to fully understand the rigidity of all generic frameworks (G, p).

It is clear that (the vertex set of) each rigid component of G is contained in a rigid cluster of G. In general G can have rigid clusters which are not vertex sets of rigid components, see Figure 3.[2] Jacobs [11] has conjectured that the rigid clusters of G are the same as the vertex sets of the rigid components of G when G is a molecular graph[3].

Conjecture 5.1. *Let $G = (V, E)$ be a graph and $U \subseteq V$. Then U is a rigid cluster of G^2 if and only if $G^2[U]$ is a rigid component of G^2.*

Let G be a graph of minimum degree at least two and $\mathcal{C}$ be the set of rigid components of G^2. The truth of Conjectures 2.6 and 5.1 would imply that $r(G^2) = val(\mathcal{C})$. Thus Conjecture 3.5, and hence also Conjectures 1.1 and 1.2, would follow from Conjectures 2.6 and 5.1.

In order to verify Conjecture 5.1, we need to show that $r(G^2 + uv) = r(G^2)$ if and only if u, v belong to the same rigid component of G^2. It seems difficult to verify this

[2]Note that the graph on Figure 3 is not a square. This follows, for example, from the simple observation that if $H = G^2$ for some graph G and $H - \{u, v\}$ is disconnected for some pair $u, v \in V(G)$, then we would have $uv \in E(H)$.

[3]This conjecture is actually a combination of two statements [11, Observation 3.1, Theorem 4.3] whose proofs are incomplete.

even if we assume that the Molecular Conjecture is true, since the graph $G^2 + uv$ need not be a molecular graph.

6 Algorithmic aspects

There is an important consequence of Corollary 4.4 from the algorithmic point of view. The brick partition can be found in polynomial time (see below). Thus, provided Conjecture 1.1 is true, we obtain a polynomial time algorithm for finding (the vertex sets of) all rigid components of G^2. This algorithms runs on $5G$.

Jacobs [11] has an algorithm, which runs on G^2, and identifies its rigid components (see also [12]). However, there is no rigorous proof for its correctness, even if we assume that Conjecture 1.1 is true.

The fact that the brick partition of a graph can be computed in polynomial time can be seen from the following more general argument. Given a multigraph $H = (V, E)$ we define H to be *k-strong*, for a positive integer k, if H has k edge-disjoint spanning trees. The *k-brick partition* of H is the partition of V into the vertex sets of the maximal k-strong subgraphs of H. To find the k-brick partition first find a maximum size subgraph $H' = (V, I)$ of H whose edge-set can be decomposed into k forests. This is the same as finding a basis in matroid $\mathcal{M}_k(H)$, which is the matroid union of k copies of the cycle matroid of H (see [4] for an efficient algorithm).

Since $C - e$ is k-strong for all $e \in E(C)$, for all circuits C of $\mathcal{M}_k(H)$ (c.f. [18, Proposition A.1.1]), it is easy to see that the k-brick partitions of H' and H are the same. Since I is independent in $\mathcal{M}_k(H)$, we have $|E_{H'}(X)| \leq k|X| - k$ for all nonempty $X \subseteq V$. Furthermore, finding the k-brick of H' containing a specified edge $uv \in I$ is then equivalent to finding a maximal subset $B \subseteq V$ which contains u, v and satisfies $|E_{H'}(B)| = k|B| - k$. This subroutine is easy to implement by maximum flow (or bipartite matching, or in-degree constrained orientation) algorithms. There exist more efficient methods, where the basis I and the k-brick partition of H are built up simultaneously. We omit the details and refer the reader to [14, Chapter 51] for a detailed survey and [1, 22] for the orientation-based approach and more references.

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