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Rank and independence in the rigidity matroid of molecular graphs

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Abstract

In this paper we consider the 3-dimensional rigidity matroid 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 independence (or more generally, computing the rank) in the rigidity matroids of squares of graphs may be tractable by combinatorial methods. We give sufficient conditions for independence and upper bounds on the rank of these matroids. In particular, we give a self-contained proof for the necessity part of the bar-and-joint version of the Molecular Conjecture. Our proofs are based on new structural results on forest covers of graphs as well as extensions of some basic techniques of combinatorial rigidity.

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 [7, 22] for the definition of $\mathcal{R}(G)$.) We denote the rank function of $\mathcal{R}(G)$ by r_G and $r_G(E)$ by $r(G)$. The following upper bound on r_G is due to Gluck.

Lemma 1.1. *[4] Let $G = (V, E)$ be a graph on at least three vertices. Then $r(G) \leq 3|V| - 6$.*

A graph $G = (V, E)$ is said to be *rigid* if either $G = K_2$ 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, 5, 6, 7, 8, 22].

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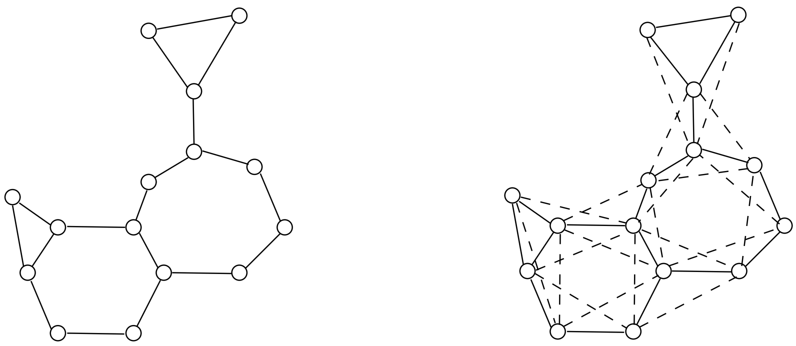

Figure 1: A graph G and its square G^2.

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 [19]. The Molecular Conjecture, due to Tay and Whiteley [18, Conjecture 1], see also [11, 22, 23, 24, 25, 26], indicates that the problem of determining when molecular graphs are rigid may be significantly easier than the problem for arbitrary graphs. This conjecture appears in the literature in several different forms, and is typically formulated in terms of 'body-and-hinge frameworks'. [1]

In this paper we shall be concerned with bar-and-joint frameworks. Conjectures 1.2 and 1.3 below are the bar-and-joint versions of the Molecular Conjecture. (We have not been able to find them explicitly in the literature.)

[1]The conjecture is related to four different realizations of a multigraph in 3-space: a *body-and-bar framework*, in which vertices are represented by rigid bodies and edges by bars attached to the corresponding pair of bodies at universal joints; a *body-and-hinge framework*, in which vertices are represented by rigid bodies and edges by hinges attached to the corresponding pair of bodies; a *molecular framework*, which is a body-and-hinge framework in which the lines containing the hinges incident to each body are constrained to meet at a common point; a *bar-and-joint framework*, in which vertices are represented by universal joints and edges by bars attached to the corresponding pair of joints. The body-and-bar and bar-and-joint representations each define a matroid on the edge set of the multigraph. Tay [16] showed that a multigraph H is rigid as a generic body-and-bar framework if and only if H has six edge-disjoint spanning trees. Indeed, Tay's result implies that the generic body-and-bar matroid of H is equal to the matroid union of six copies of the cycle matroid of H. The generic body-and-hinge framework and the generic molecular framework for a graph G are each equivalent to a special kind of non-generic body-and-bar framework for the multigraph $5G$. Tay [17] and Whiteley [21] independently showed that a graph G is rigid as a generic body-and-hinge framework if and only if $5G$ has six edge-disjoint spanning trees (this result was first announced in [18]). They also conjectured in [18, Conjecture 1] that G is rigid as a generic molecular framework if and only if G is rigid as a generic body-and-hinge framework. By the preceding result, this is equivalent to the conjecture that G is rigid as a generic molecular framework if and only if $5G$ has six edge-disjoint spanning trees. Whiteley [25] has recently shown that a graph G of minimum degree at least two is rigid as a generic molecular framework if and only if G^2 is rigid as a generic bar-and-joint framework. It follows that the above mentioned Molecular Conjecture of Tay and Whiteley is equivalent to Conjecture 1.2 in this paper. See [22, 26] for definitions and more details on these different frameworks.

Conjecture 1.2. (Molecular Conjecture) *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 1.2 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 1.3. (Molecular Conjecture, defect form) *Let $G = (V, E)$ be a graph with minimum degree at least two. Then*

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

Part (b) of the following theorem shows that Conjecture 1.3 implies Conjecture 1.2. (In Section 5 we shall prove that the reverse implication also holds.)

Theorem 1.4. *[12, 13, 20] Let $H = (V, E)$ be a multigraph and let k be a positive integer. Then*
(a) the maximum size of the union of k forests in H is equal to the minimun value of

$$e_H(\mathcal{P}) + k(|V| - |\mathcal{P}|) \tag{2}$$

taken over all partitions $\mathcal{P}$ of V;
(b) H contains k edge-disjoint spanning trees if and only if

$$e_H(\mathcal{P}) \geq k(|\mathcal{P}| - 1)$$

for all partitions $\mathcal{P}$ of V;
(c) the edge set of H can be covered by k forests if and only if

$$|E(H[X])| \leq k(|X| - 1)$$

for each nonempty subset X of V.

Theorem 1.4(a) appears in [15, Chapter 51]. It follows easily from the matroid union theorem of Nash-Williams [14] and Edmonds [1], which determine the rank function of the union of k matroids, by applying this theorem to the matroid $\mathcal{M}_k(H)$ which is the union of k copies of the cycle matroid of H. Part (a) implies parts (b) and (c), which are well-known results of Tutte [20] and Nash-Williams [12], and Nash-Williams [13], respectively.

The minimum value of (2) is equal to $r_k(E)$, where r_k denotes the rank function of $\mathcal{M}_k(H)$. Thus Conjecture 1.3 states that $r(G^2) = r_6(5G) - 3|V|$. Note, however, that the independence of $E(G^2)$ in $\mathcal{R}(G^2)$ is, in general, not equivalent to the independence of $E(5G)$ in $\mathcal{M}_6(5G)$, as shown for example by taking $G = C_3, C_4$.

The rest of the paper is organized as follows. In Section 2 we recall some basic results from combinatorial rigidity. Section 3 contains a proof that the right hand side of (1) gives an upper bound on $r(G^2)$. We give new structural results on forest covers and extend some basic operations in combinatorial rigidity in Sections 4 and 7, respectively. In Section 5 we show that Conjecture 1.2 implies Conjecture 1.3. In Sections 6 and 8 we give various conditions for $E(G^2)$ to be independent in $\mathcal{R}(G^2)$.

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* if E is independent in $\mathcal{R}(G)$.

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

Lemma 2.1. *[22, Lemma 9.1.3] Let $H = (V, E)$ be a graph and $v_1, v_2, \dots v_s$ 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. *[22, 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.

A *cover* of $G = (V, E)$ 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 $|X_i \cap X_j| \le t$ for all $1 \le i < j \le m$. For $X_i \in \mathcal{X}$ let $f(X_i) = 1$ if $|X_i| = 2$ and $f(X_i) = 3|X_i| - 6$ if $|X_i| \ge 3$. Let $H(\mathcal{X})$ be the set of all pairs of vertices uv such that $X_i \cap X_j = \{u, v\}$ for some $1 \le i < j \le m$. For each $uv \in H(\mathcal{X})$ let $h(uv)$ be the number of sets X_i in $\mathcal{X}$ such that $\{u, v\} \subseteq X_i$ and put

$$val(\mathcal{X}) = \sum_{X \in \mathcal{X}} f(X) - \sum_{uv \in H(\mathcal{X})} (h(uv) - 1).$$

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

Lemma 2.3. *[7, Lemma 3.2] Let $G = (V, E)$ be a graph, and $\mathcal{X}$ be an independent cover of G. Then $r(G) \leq val(\mathcal{X})$.*

3 The upper bound

In this section we give a direct proof that the right hand side of (1) gives an upper bound on $r(G^2)$. Given a graph $G = (V, E)$, we say that a partition $\mathcal{P}$ of V is a *tight partition of* G if $\text{def}_G(\mathcal{P}) = \text{def}(G)$. We say that $\mathcal{P}$ *induces a cycle of length* k *in* G if there exist distinct classes $P_1, P_2, \dots, P_k \in \mathcal{P}$ and distinct edges $e_1, e_2, ..., e_k \in E$ such that $e_i \in E_G(P_i, P_{i+1})$ for $1 \leq i \leq k-1$ and $e_k \in E_G(P_k, P_1)$.

Lemma 3.1. *Let $G = (V, E)$ be a graph and $\mathcal{P}$ be a tight partition of V. Let $\mathcal{Q} \subseteq \mathcal{P}$ with $|\mathcal{Q}| \geq 2$, $P' = \cup_{P \in \mathcal{Q}} P$ and $H = G[P']$. Then*
(a) $def_H(\mathcal{Q}) \geq 0$ and $\mathcal{P}$ does not induce a cycle of length less than six in G.
(b) Furthermore, if $\mathcal{P}$ is chosen such that $|\mathcal{P}|$ is as small as possible, then $def_H(\mathcal{Q}) \geq 1$ and $\mathcal{P}$ does not induce a cycle of length less than seven in G.

Proof: Let $\mathcal{R} = (\mathcal{P} - \mathcal{Q}) \cup \{P'\}$. Then

$$\text{def}_G(\mathcal{P}) = \text{def}_G(\mathcal{R}) + \text{def}_H(\mathcal{Q}).$$

Since $\mathcal{P}$ is a tight partition of G we have $\text{def}_G(\mathcal{P}) \geq \text{def}_G(\mathcal{R})$. Hence $\text{def}_H(\mathcal{Q}) \geq 0$. In particular, if $2 \leq |\mathcal{Q}| \leq 5$, we have $e_G(\mathcal{Q}) \leq \frac{6}{5}(|\mathcal{Q}| - 1) < |\mathcal{Q}|$. Thus $\mathcal{P}$ does not induce a cycle of length less than six in G and (a) holds.

Now suppose that $\text{def}_H(\mathcal{Q}) = 0$. Then $\text{def}_G(\mathcal{P}) = \text{def}_G(\mathcal{R})$. Thus $\mathcal{R}$ is a tight partition of G with $|\mathcal{R}| = |\mathcal{P}| - |\mathcal{Q}| + 1$. Hence, if $\mathcal{P}$ is chosen such that $|\mathcal{P}|$ is as small as possible, then we must have $\text{def}_H(\mathcal{Q}) \geq 1$. The implication concerning cycles induced by $\mathcal{P}$ follows as in the previous paragraph. •

Theorem 3.2. *Let $G = (V, E)$ be a graph of minimum degree at least two. Then*

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

Proof: Since $r(G^2) \leq 3|V| - 6$ by Lemma 1.1, we may assume that $\text{def}(G) \geq 1$. Let $\mathcal{P} = \{P_1, P_2, ..., P_t\}$ be a tight partition of V. Since $\text{def}(G) \geq 1$, we must have $t \geq 2$. By Lemma 3.1(a), $\mathcal{P}$ does not induce a cycle of length less than six in G. In particular, $e_G(\{P_i, P_j\}) \leq 1$ for all $1 \leq i < j \leq t$.

Let $X_i = P_i \cup N_G(P_i)$ for $1 \leq i \leq t$ and let $\mathcal{X} = \{X_1, ..., X_t\}$. It is easy to see that $\mathcal{X}$ is a cover of G^2. Furthermore, since $e_G(\{P_i, P_j\}) \leq 1$ for $1 \leq i < j \leq t$, and G has minimum degree at least two, we have $|X_i| = |P_i| + d_G(P_i)$ and $|X_i| \geq 3$ for $1 \leq i \leq t$. By using the fact that $\mathcal{P}$ does not induce cycles of length two, three or four in G, it is also easy to verify that $\mathcal{X}$ is a 2-thin cover with $H(\mathcal{X}) = \{uv : uv \in E_G(\mathcal{P})\}$ and $h(uv) = 2$ for all $uv \in H(\mathcal{X})$.

We claim that $K = (V, H(\mathcal{X})) = (V, E_G(\mathcal{P}))$ is M-independent, and hence $\mathcal{X}$ is an independent cover of G^2. To see this consider a nonempty subset $Z \subseteq V$. If $Z \subseteq P_i$

holds for some $1 \le i \le t$ then $i_K(Z) = 0$. Now suppose that Z intersects at least two members of $\mathcal{P}$ and let $\mathcal{Q} = \{P_i \in \mathcal{P} : Z \cap P_i \neq \emptyset\}$. By Lemma 3.1(a) we have

$$5i_K(Z) \le 5e_G(\mathcal{Q}) \le 6(|\mathcal{Q}| - 1) \le 6(|Z| - 1).$$

Hence $i_K(Z) \le \frac{6}{5}(|Z| - 1)$ for all nonempty $Z \subseteq V$.

Thus K is sparse: every subgraph of K has average degree less than three, and hence has a vertex of degree at most two. This implies that K can be obtained from a collection of disjoint edges (which is M-independent) by a sequence of 0-extensions. Thus K is M-independent by Lemma 2.1.

Since $\mathcal{X}$ is an independent cover of G^2, we can use Lemma 2.3 to deduce that

$$\begin{aligned} r(G^2) &\le val(\mathcal{X}) = \sum_{i=1}^{t} f(X_i) - \sum_{uv \in H(\mathcal{X})} (h(uv) - 1) \\ &= \sum_{i=1}^{t} (3|X_i| - 6) - |E_G(\mathcal{P})| = \sum_{i=1}^{t} 3(|P_i| + d_G(P_i)) - |E_G(\mathcal{P})| - 6t \\ &= 3|V| + 6|E_G(\mathcal{P})| - |E_G(\mathcal{P})| - 6t = 3|V| + 5e_G(\mathcal{P}) - 6t \\ &= 3|V| - 6 - \mathrm{def}(\mathcal{P}) = 3|V| - 6 - \mathrm{def}(G), \end{aligned}$$

as required. •

Remark Suppose that $G = (V, E)$ is a graph of minimum degree at least two and let $\mathcal{P}$ be a tight partition of V. The truth of Conjecture 1.3 would imply that $r(G^2) = \mathrm{def}_G(\mathcal{P})$. Thus we would have $r(G^2) = val(\mathcal{X})$ where $\mathcal{X}$ is the independent 2-thin cover of G^2 constructed from $\mathcal{P}$ as in the proof of Theorem 3.2. Hence Conjecture 1.3 would imply that the upper bound on $r(H)$ given by Lemma 2.3 holds with equality for some independent 2-thin cover of H, when $H = G^2$. This is not the case when H is an arbitrary graph, see [8, Example 3].

We close this section by showing that, if true, Conjecture 1.3 could be used to determine the rank of squares of all graphs, not just graphs of minimum degree at least two. Let $G = (V, E)$ be a connected graph on at least two vertices and let $L(G)$ denote the set, and $l(G)$ the number of vertices of degree one in G. Let G_{core} be the maximal subgraph of G of minimum degree at least two. Note that G_{core} is empty if and only if G is a tree, and $G = G_{core}$ if and only if $L(G)$ is empty. Part (a) of the next lemma is due to Franzblau [3].

Lemma 3.3. *Let $G = (V, E)$ be a connected graph on at least two vertices. Then*
(a) if G is a tree then $r(G^2) = 2|V| - 5 + l(G)$;
(b) if G is not a tree then

$$r(G^2) = r((G_{core})^2) + 2|V(G - G_{core})| + l(G).$$

Proof: Induction on $|V|$. The theorem is trivially true if $|V| = 2$ or $L(G) = \emptyset$, so we may assume that $L(G) \neq \emptyset$ and $|V| \ge 3$. Let $v \in L(G)$, let $H = G - v$, and let u be the neighbour of v in G. If $d_G(u) \ge 3$, then $r(G^2) = r(H^2) + 3$ (by Lemma

2.1), $G_{core} = H_{core}$ and $l(G) = l(H) + 1$. On the other hand, if $d_G(u) = 2$ then $r(G^2) = r(H^2) + 2$ (by Lemma 2.1), $G_{core} = H_{core}$ and $l(G) = l(H)$. In both cases, the lemma follows by applying induction to H. •

4 Bricks and superbricks

We say that a graph G is *strong* if $5G$ has six edge-disjoint spanning trees. Equivalently, by Theorem 1.4(b), G is strong if $\mathrm{def}(G) = 0$.

Lemma 4.1. *Let $G = (V, E)$ be a graph, and $\mathcal{P}$ be a tight partition of G. Choose $P \in \mathcal{P}$ and let $H = G[P]$. Then:*
(a) H is strong;
(b) if $\mathcal{P}$ is chosen such that $|\mathcal{P}|$ is as large as possible, then $\{P\}$ is the only tight partition of H.

Proof: Let $\mathcal{Q}$ be a tight partition of H and $\mathcal{R} = (\mathcal{P} - \{P\}) \cup \mathcal{Q}$. Then $\mathcal{R}$ is a partition of V and

$$\mathrm{def}_G(\mathcal{R}) = \mathrm{def}_G(\mathcal{P}) + \mathrm{def}_H(\mathcal{Q}).$$

Since $\mathcal{P}$ is a tight partition of G we have $\mathrm{def}_H(\mathcal{Q}) \leq 0$. Since $\mathcal{Q}$ is a tight partition of H, $\mathrm{def}_H(\mathcal{Q}) \geq 0$. Thus $\mathrm{def}_H(\mathcal{Q}) = 0$ and H is strong. Furthermore, $\mathrm{def}_G(\mathcal{R}) = \mathrm{def}_G(\mathcal{P})$. Thus, if $\mathcal{P}$ is chosen such that $|\mathcal{P}|$ is as large as possible, we must have $|\mathcal{Q}| = 1$ and $\mathcal{Q} = \{P\}$. •

A subgraph H of a graph G is said to be a *brick* of G if H is a maximal strong subgraph of G. Thus bricks are induced subgraphs.

Lemma 4.2. *Let $G = (V, E)$ be a graph, let $X_1, X_2 \subseteq V$ with $X_1 \cap X_2 \neq \emptyset$ and suppose that $G[X_1]$ and $G[X_2]$ are strong. Then $G[X_1 \cup X_2]$ is strong.*

Proof: For a contradiction suppose that $H = G[X_1 \cup X_2]$ is not strong, and let $\mathcal{P} = \{P_1, P_2, ..., P_t\}$ be a tight partition of H for which $|\mathcal{P}|$ is as small as possible. Since $\mathrm{def}(H) \geq 1$, we have $t \geq 2$. Let $\mathcal{Q}_i = \{P_j \in \mathcal{P} : X_i \cap P_j \neq \emptyset\}$ and $\mathcal{Q}'_i = \{X_i \cap P_j : P_j \in \mathcal{Q}_i\}$, for $i = 1, 2$. Suppose that $|\mathcal{Q}_i| = |\mathcal{Q}'_i| \geq 2$ for some $i \in \{1, 2\}$. Then

$$6(|\mathcal{Q}'_i| - 1) \leq 5e_{G[X_i]}(\mathcal{Q}'_i) \leq 5e_H(\mathcal{Q}_i) \leq 6(|\mathcal{Q}_i| - 1) - 1,$$

where the first inequality follows from the fact that $G[X_i]$ is strong, and the last inequality follows from Lemma 3.1(b). This contradiction implies that $|\mathcal{Q}_i| = 1$, and hence X_i is a subset of some member of $\mathcal{P}$, for $i = 1, 2$. This contradicts the fact that $\mathcal{P}$ is a partition of $X_1 \cup X_2$, $t \geq 2$, and $X_1 \cap X_2 \neq \emptyset$. Thus H is strong. •

It follows immediately that the bricks of a graph G are vertex disjoint. Since, by definition, a single vertex is strong, every vertex of G belongs to a brick, and hence we have:

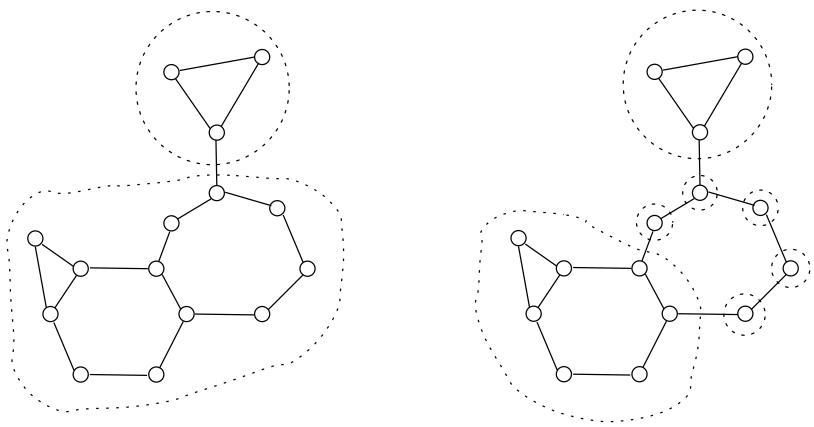

Figure 2: The brick partition and the superbrick partition of graph G.

Corollary 4.3. *The vertex sets of the bricks of a graph $G = (V, E)$ partition V.*

We shall use the term *brick partition* of G to refer to the partition of V given by the vertex sets of the bricks of G.

Lemma 4.4. *Let $G = (V, E)$ be a graph and $\mathcal{P}$ be a tight partition of V such that $|\mathcal{P}|$ is as small as possible. Then $\mathcal{P}$ is the brick partition of G.*

Proof: Let $\mathcal{B}$ be the brick partition of G. If $\mathrm{def}(G) = 0$ then G is a brick and $\mathcal{B} = \{V\} = \mathcal{P}$, so we may assume that $\mathrm{def}(G) \geq 1$. Lemma 4.1(a) implies that each of the parts in $\mathcal{P}$ induces a strong subgraph of G. Thus $\mathcal{P}$ is a refinement of $\mathcal{B}$ by Lemma 4.2. Since each part of $\mathcal{B}$ induces a strong subgraph of G, Lemma 3.1(b) now implies that $\mathcal{B} = \mathcal{P}$. •

We say that a graph $G = (V, E)$ is *superstrong* if $5G - e$ has six edge-disjoint spanning trees for all $e \in E(5G)$. Equivalently, by Theorem 1.4(b), G is superstrong if $\mathrm{def}(G) = 0$ and the only tight partition of V is $\{V\}$ itself. A subgraph H of G is said to be a *superbrick* of G if H is a maximal superstrong subgraph of G.

Lemma 4.5. *Let $G = (V, E)$ be a graph, let $X_1, X_2 \subseteq V$ with $X_1 \cap X_2 \neq \emptyset$ and suppose that $G[X_1]$ and $G[X_2]$ are superstrong subgraphs of G. Then $G[X_1 \cup X_2]$ is superstrong.*

Proof: Let $H = G[X_1 \cup X_2]$ and suppose H is not superstrong. Then we may choose $e \in E(5H)$ such that the graph $G^* = 5H - e$ does not have six edge-disjoint spanning trees. By Theorem 1.4, there exists a partition $\mathcal{P}$ of V such that $6(|\mathcal{P}|-1) - e_{G^*}(\mathcal{P}) > 0$. Choose $\mathcal{P}$ such that $6(|\mathcal{P}|-1) - e_{G^*}(\mathcal{P})$ is as large as possible and, subject to this condition, $|\mathcal{P}|$ is as small as possible. Using the same argument as in the proof of Lemma 3.1(b), we may deduce that $6(|\mathcal{Q}| - 1) - e_{G^*}(\mathcal{Q}) > 0$ for all $\mathcal{Q} \subseteq \mathcal{P}$ with $|\mathcal{Q}| \geq 2$. We may now use the fact that $5G[X_i] - e$ has six edge-disjoint spanning trees for $i = 1, 2$ to obtain a contradiction as in the proof of Lemma 4.2. •

It follows immediately that the superbricks of a graph G are vertex disjoint. Since, by definition, a single vertex is superstrong, every vertex of G belongs to a superbrick, and hence we have:

Corollary 4.6. *The vertex sets of the superbricks of a graph $G = (V, E)$ partition V.*

We shall use the term *superbrick partition* of G to refer to the partition of V given by the vertex sets of the superbricks of G.

Lemma 4.7. *Let G be a graph and $\mathcal{P}$ be a tight partition of V such that $|\mathcal{P}|$ is as large as possible. Then $\mathcal{P}$ is the superbrick partition of G.*

Proof: Let $\mathcal{S}$ be the superbrick partition of G. If $|\mathcal{P}| = 1$ then G is a superbrick and $\mathcal{S} = \{V\} = \mathcal{P}$, so we may assume that $|\mathcal{P}| \geq 2$. Lemma 4.1(b) implies that each of the parts in $\mathcal{P}$ induces a superstrong subgraph of G. Thus $\mathcal{P}$ is a refinement of $\mathcal{S}$ by Lemma 4.5. Since the union of two or more parts of $\mathcal{P}$ induces a subgraph of G which is not superstrong by Lemma 3.1(a), we may deduce that $\mathcal{S} = \mathcal{P}$. •

We say that a superstrong graph G is *minimally superstrong* if $G - e$ is not superstrong for all $e \in E(G)$.

Lemma 4.8. *Let $G = (V, E)$ be a minimally superstrong graph and let H be a superstrong subgraph of G. Then H is minimally superstrong.*

Proof: Let $e \in E(H)$ and consider the superbrick partition $\mathcal{S} = \{P_1, P_2, ..., P_t\}$ of $G - e$. Since G is minimally superstrong, $t \geq 2$ and the endvertices of e belong to different classes of $\mathcal{S}$. Let $\mathcal{Q} \subseteq \mathcal{S}$ consist of those classes of $\mathcal{S}$ which contain at least one vertex of H. If $H - e$ is superstrong, we must have $5e_H(\mathcal{Q}) \geq 6(|\mathcal{Q}| - 1) + 1$. Since $\mathcal{S}$ is a tight partition of V by Lemma 4.7, this contradicts Lemma 3.1(a). Thus $H - e$ is not superstrong, as claimed. •

The results of this section hold in a much more general context. Let q be a positive rational number and k, h be positive integers such that $q = k/h$. Given a multigraph $G = (V, E)$ we define G to be *q-strong* if hG has k edge-disjoint spanning trees. By Theorem 1.4, G is q-strong if and only if $he_G(\mathcal{P}) \geq k(|\mathcal{P}| - 1)$ for all partitions $\mathcal{P}$ of V, and hence the definition of q-strong does not depend on which integers k, h we use to represent q. We may proceed as above to define the *q-bricks*, the *q-superbricks*, the *q-brick partition*, and the *q-superbrick partition* of G.[2] (When $q = k$ is a positive integer, the concepts of k-strong and k-superstrong have already been considered by Frank and Király [2], where they are referred to as k-tree-connected and $(k, 1)$-tree-connected, respectively.) By using well-known algorithms for packing trees, or more generally, packing independent sets in a matroid (see [15] for a survey) it is easy to obtain efficient algorithms for testing whether a multigraph G is q-(super)strong, and for determining the q-(super)brick partition of G.

[2] This general approach would have simplified the proof of Lemma 4.5, but would not have been relevant to the rest of the paper.

5 The equivalence of Conjectures 1.2 and 1.3

Lemma 5.1. *Conjectures 1.2 and 1.3 are equivalent.*

Proof: The fact that Conjecture 1.3 implies Conjecture 1.2 follows immediately from Theorem 1.4(b), as we noted earlier.

Suppose Conjecture 1.2 holds and let $G = (V, E)$ be a graph of minimum degree at least two. We show that Conjecture 1.3 holds for G by induction on $\mathrm{def}(G)$. If $\mathrm{def}(G) = 0$, then Theorem 1.4(b) implies that $5G$ has six edge-disjoint spanning trees. Since Conjecture 1.2 holds, G^2 is rigid and hence $r(G^2) = 3|V| - 6$. Thus Conjecture 1.3 holds for G. Hence we may assume that $\mathrm{def}(G) \geq 1$. Let $\mathcal{B}$ be the brick partition of G. Since $\mathrm{def}(G) \geq 1$, we have $|\mathcal{B}| \geq 2$. Choose two vertices u, u' belonging to distinct bricks $B, B' \in \mathcal{B}$, respectively.

Let G_1 be the graph obtained from G by attaching an ear $P = ux_1x_2x_3x_4u'$ of length five at u, u'.

Claim 5.2. *def*$(G_1) =$ *def*$(G) - 1$.

Proof: Consider the brick partition $\mathcal{B}_1$ of G_1. Since each brick with at least three vertices has minimum degree two, the vertices x_1, x_2, x_3, x_4 either each occur as singleton bricks of G_1, or are all contained in the same brick of G_1. Since the bricks of G are maximal strong subgraphs of G, it follows that $\mathcal{B}_1 = \mathcal{P}$ or $\mathcal{B}_1 = \mathcal{P}'$, where

$$\mathcal{P} = \mathcal{B} \cup \{\{x_1\}, \{x_2\}, \{x_3\}, \{x_4\}\},$$

and

$$\mathcal{P}' = (\mathcal{B} - \mathcal{Q}) \cup \{(\bigcup_{B_i \in \mathcal{Q}} B_i) \cup \{x_1, x_2, x_3, x_4\}\},$$

for some $\mathcal{Q} \subseteq \mathcal{B}$ with $B, B' \in \mathcal{Q}$. We have

$$\begin{aligned} \mathrm{def}_{G_1}(\mathcal{P}) &= 6(|\mathcal{P}| - 1) - 5e_{G_1}(\mathcal{P}) = 6(|\mathcal{B}| + 4 - 1) - 5(e_G\mathcal{B} + 5) \\ &= \mathrm{def}_G(\mathcal{B}) - 1 = \mathrm{def}(G) - 1. \end{aligned}$$

On the other hand, if we let $\mathcal{R} = (\mathcal{B} - \mathcal{Q}) \cup \left\{\bigcup_{B_i \in \mathcal{Q}} B_i\right\}$ then $\mathcal{R}$ partitions V, $|\mathcal{R}| < |\mathcal{B}|$ since $|\mathcal{Q}| \geq 2$, and

$$\mathrm{def}_{G_1}(\mathcal{P}') = \mathrm{def}_G(\mathcal{R}) < \mathrm{def}_G(\mathcal{B}) = \mathrm{def}(G),$$

by Lemma 4.4. Thus $\mathrm{def}_{G_1}(\mathcal{B}_1) = \mathrm{def}(G) - 1$. The claim now follows since $\mathrm{def}(G_1) = \mathrm{def}_{G_1}(\mathcal{B}_1)$. •

It follows from Claim 5.2 that we may apply induction to G_1 and deduce that

$$\begin{aligned} r(G_1^2) &= 3|V(G_1)| - 6 - \mathrm{def}(G_1) = 3(|V| + 4) - 6 - (\mathrm{def}(G) - 1) \\ &= 3|V| - 6 - \mathrm{def}(G) + 13. \end{aligned} \quad (3)$$

Consider the graph H obtained from G by adding the vertices x_1, x_4 and edges $ux_1, u'x_4$. Since the neighbour sets of u and u' in H^2 each induce complete (and hence rigid) subgraphs with at least three vertices, we have $r(H^2) = r(G^2) + 6$. This gives

$$r(G_1^2) \leq r(H^2) + |E(G_1^2) - E(H^2)| = (r(G^2) + 6) + 7 = r(G^2) + 13. \qquad (4)$$

Combining (3) and (4), we obtain $3|V| - 6 - \mathrm{def}(G) + 13 = r(G_1^2) \leq r(G^2) + 13$. Hence $r(G^2) \geq 3|V| - 6 - \mathrm{def}(G)$. Theorem 3.2 now implies that $r(G^2) = 3|V| - 6 - \mathrm{def}(G)$. Hence Conjecture 1.3 holds for G. •

6 Independent squares

Recall that a graph $G = (V, E)$ is *M-independent* if $r(G) = |E|$. We say that a graph G is *Laman* if for all subgraphs of G induced by a subset $X \subseteq V$ with $|X| \geq 3$, the number of edges is at most $3|X| - 6$. Lemma 1.1 implies that if G is M-independent then G is Laman. Jacobs [10] conjectures that the reverse implication also holds for squares of graphs. [3]

Conjecture 6.1. *Let G be a graph. Then G^2 is M-independent if and only if G^2 is Laman.*

We will show that Conjecture 6.1 would follow from Conjecture 1.3. We use the following two results.

Lemma 6.2. *Let $G = (V, E)$ be a graph such that G^2 is Laman. Then each vertex of G has degree at most three.*

Proof: Choose $v \in V$. Then $G^2[N_G(v) \cup \{v\}]$ is a complete graph on $d_G(v) + 1$ vertices. Since the complete graph K_n is Laman only when $n \leq 4$, we have $d_G(v) \leq 3$. •

Theorem 6.3. *Suppose that G has minimum degree at least two and G^2 is Laman. Then $|E(G^2)| \leq 3|V(G)| - 6 -$ def(G).*

Proof: We may assume that $\mathrm{def}(G) \geq 1$, since the theorem trivially holds for Laman graphs with deficiency zero. Let $\mathcal{P} = \{P_1, P_2, ..., P_t\}$ be a tight partition of V. Since $\mathrm{def}(G) \geq 1$, we must have $t \geq 2$.

An edge $uw \in E(G^2)$ is called a *cross edge*, if $uw \in E_{G^2}(\mathcal{P})$ and $uw \notin E(G)$. Lemma 3.1(a) implies that for every cross edge uw there is a unique pair uv, vw of adjacent edges of G which 'implies' uw. Clearly, at least one of the edges uv, vw must also belong to $E_{G^2}(\mathcal{P})$. We say that the cross edge uw is *normal* (*special*) if precisely one (respectively, both) of the edges uv, vw connect distinct members of $\mathcal{P}$. Let C_n

[3] He states the conjecture as a result, [10, Proposition 4.9], but his proof is incomplete since it assumes the truth of [10, Observation 3.1] for which no proof is yet known.

and C_s denote the number of normal and special cross edges of G^2, respectively. A normal edge f is *rooted at* P_i if one of the two edges of G that 'imply' f is induced by P_i.

It follows from Lemma 4.1(a) that $G[P_i]$ is strong, and hence for all $1 \leq i \leq t$ either $|P_i| = 1$, or $|P_i| \geq 3$ and $d_{G[P_i]}(v) \geq 2$ holds for all $v \in P_i$. Let $\mathcal{P}_s = \{P_i : P_i \in \mathcal{P}, |P_i| = 1\}$ and let $\mathcal{P}_b = \{P_i : P_i \in \mathcal{P}, |P_i| \geq 3\}$.

Consider a set $P_i \in \mathcal{P}_b$ and an edge $uv \in E_{G^2}(\mathcal{P})$ with $v \in P_i$. Since G^2 is Laman, $d_G(v) \leq 3$ by Lemma 6.2. Thus, since $d_{G[P_i]}(v) \geq 2$, there are exactly two normal cross edges which are 'implied' by pairs uv, vw, for some $w \in P_i$. Hence the number of normal cross edges rooted at P_i is $2d_G(P_i)$. It also follows that if a pair of edges 'implies' a special cross edge then their common vertex cannot belong to P_i.

Now consider a set $P_j \in \mathcal{P}_s$. By Lemma 3.1(a) $G^2[N_G(P_j)]$ is a complete subgraph consisting of special cross edges, and all special cross edges can be obtained this way for a unique member of $\mathcal{P}_s$. Since $d_G(v) \in \{2, 3\}$ for all $v \in V$, we have

$$|E(G^2[N_G(P_j)])| = 2d_G(P_j) - 3. \tag{5}$$

By using these observations we can count the normal edges at their roots and special edges in the neighbourhoods of the singleton members of $\mathcal{P}$. Thus

$$C_n = \sum_{P_i \in \mathcal{P}_b} 2d_G(P_i), \tag{6}$$

$$C_s = \sum_{P_j \in \mathcal{P}_s} |E(G^2[N_G(P_j)])|. \tag{7}$$

Using (5), (6), (7), and the fact that G^2 is Laman we obtain:

$$\begin{aligned}
|E(G^2)| &= \sum_{i=1}^{t} |E(G^2[P_i])| + e_G(\mathcal{P}) + C_n + C_s \\
&\leq \sum_{P_i \in \mathcal{P}_b} (3|P_i| - 6) + e_G(\mathcal{P}) + \sum_{P_i \in \mathcal{P}_b} 2d_G(P_i) + \sum_{P_j \in \mathcal{P}_s} |E(G^2[N_G(P_j)])| \\
&= \sum_{i=1}^{t} (3|P_i| - 6) + e_G(\mathcal{P}) + \sum_{i=1}^{t} 2d_G(P_i) \\
&= 3|V| - 6t + 5e_G(\mathcal{P}) = 3|V| - 6 - \mathrm{def}(\mathcal{P}) = 3|V| - 6 - \mathrm{def}(G),
\end{aligned}$$

as claimed. •

We can now show that Conjecture 6.1 would follow from Conjecture 1.3. To see this suppose, for a contradiction, that G^2 is Laman but $r(G^2) < |E(G^2)|$. Since for graphs G of maximum degree at most three G^2 is M-independent if and only if $(G_{core})^2$ is M-independent, we may assume that G has minimum degree at least two. By using Theorem 6.3 and assuming that Conjecture 1.3 holds for G, this gives $|E(G^2)| \leq 3|V| - 6 - \mathrm{def}(G) = r(G^2) < |E(G^2)|$, a contradiction.

We next show that the superbrick partition of a graph G can be used to determine when G^2 is Laman. More precisely we will show in Theorem 6.8 below that G^2 is Laman if and only if each vertex of G has degree at most three and each superbrick of G has at most four vertices.

Lemma 6.4. *Let $G = (V, E)$ be a superstrong graph with at least five vertices and with maximum degree $\Delta \leq 3$. Then $|E(G^2)| \geq 3|V| - 5$.*

Proof: Without loss of generality, we may assume that G is minimally superstrong. By Lemma 4.8 this implies that every superstrong subgraph H of G is minimally superstrong. We may deduce the following claim concerning cycles in G. We say an edge uv is a *chord* of a cycle C of G if $u, v \in V(C)$ and $uv \notin E(C)$. It is a *long chord* of C if it is a chord and u and v have distance at least three around C.

Claim 6.5. *(a) No cycle of length at most five in G can have a chord.*
(b) No cycle of length at most seven in G can have two chords.
(c) No cycle of length eight in G can have two chords, at least one of which is long.
(d) No cycle C of length at most seven in G can contain three vertices with a common neighbour in $G - C$.

Proof: This follows since a cycle of length at most five, a cycle of length at most seven with a chord, a cycle of length eight with a long chord, and the graph obtained from a cycle of length at most seven by joining a new vertex to two non-adjacent vertices of the cycle, are all superstrong. •

Consider the following four graphs: $H_1 = K_3$; $H_2 = K_{2,2}$; $H_3 = K_{2,3}$; H_4 is obtained from a cycle of length six by adding a long chord. We will refer to a subgraph of G which is isomorphic to H_i for some $1 \leq i \leq 4$ as a H_i-subgraph of G. Since H_i is superstrong for all $1 \leq i \leq 4$, each H_i-subgraph of G is an induced subgraph. A subgraph F of G is *special* if F is a H_i-subgraph of G for some $1 \leq i \leq 4$, and F is not a proper subgraph of a H_j-subgraph of G for all $1 \leq j \leq 4$. The proof of the next claim is rather long and tedious. A reader who is not interested in the details could skip it without compromising their understanding of the rest of the proof.

Claim 6.6. *Any two special subgraphs of G are vertex disjoint.*

Proof: We proceed by contradiction. Suppose $F_1 = (V_1, E_1)$ and $F_2 = (V_2, E_2)$ are special subgraphs of G and $V_1 \cap V_2 \neq \emptyset$. Note that since $\Delta \leq 3$ and each special subgraph has minimum degree two, $F_1 \cap F_2$ has minimum degree at least one.

Suppose $F_1 = K_3$. Since F_2 is an induced subgraph of G we have $V_1 \cap V_2 = \{u, v\}$ and $uv \in E_2$. Since all edges of F_2 are contained in a cycle of length at most four, we have a cycle of length at most five with a chord in $F_1 \cup F_2$. This contradicts Claim 6.5(a). Thus $F_1 \neq K_3$ and, by symmetry, $F_2 \neq K_3$.

Suppose $F_1 = K_{2,2}$. Since F_1 is not a subgraph of F_2 and F_2 is induced, we have $|V_1 \cap V_2| \leq 3$. We first consider the case when $|V_1 \cap V_2| = 3$. Then $F_1 \cap F_2$ is a path $u_1u_2u_3$ of length two and $V_1 = \{u_1, u_2, u_3, x\}$. Then u_1, u_3 have degree two in F_2. If u_2 also has degree two in F_2 then we must have $F_2 = K_{2,2}$. This would give

$F_1 \cup F_2 = K_{2,3}$ and contradict the maximality of F_1. Hence u_2 has degree three in F_2. If $F_2 = K_{2,3}$ then $F_1 \cup F_2$ is a cycle of length six with two chords, and if $F_2 = H_4$ then $(F_1 \cup F_2) - u_2$ is a cycle of length six. These alternatives contradict Claim 6.5 parts (b) and (d), respectively. Thus we have $|V_1 \cap V_2| = 2$ and $E_1 \cap E_2 = \{uv\}$, say. If $F_2 = K_{2,2}$ then $F_1 \cup F_2 = H_4$. This would contradict the maximality of F_1. Since u, v are two adjacent vertices of degree two in F_2, $F_2 \neq K_{2,3}$. Thus we must have $F_2 = H_4$. But then $F_1 \cup F_2$ is a cycle of length eight with two long chords, contradicting Claim 6.5(c). Thus $F_1 \neq K_{2,2}$ and, by symmetry, $F_2 \neq K_{2,2}$.

Suppose $F_1 = K_{2,3}$. Since F_1 is not a subgraph of F_2 we have $|V_1 \cap V_2| \leq 4$. We first consider the case when $|V_1 \cap V_2| = 4$. Since $F_1 \cap F_2$ is a subgraph of F_1, we have $F_1 \cap F_2 = K_{2,2}$ or $F_1 \cap F_2 = K_{1,3}$. The first alternative would imply that F_2 contains two independent vertices of degree two in a 4-cycle. The second alternative would imply that F_2 contains three independent vertices of degree two. Thus, in both cases, we must have $F_2 = K_{2,3}$. It is easy to see that $F_1 \cup F_2$ will contain a cycle of length six with two chords. This contradicts Claim 6.5(b). We next consider the case when $|V_1 \cap V_2| = 3$. Then $F_1 \cap F_2$ is a path $u_1u_2u_3$ of length two. Since $\Delta \leq 3$, the vertices u_1, u_3 must be non-adjacent vertices of degree two in F_1 and F_2. Furthermore u_2 must have degree three in F_1, and hence must have degree two in F_2. This is impossible since either $F_2 = K_{2,3}$ or $F_2 = H_4$, and neither of these graphs have three vertices of degree two which induce a path. Thus we must have $|V_1 \cap V_2| = 2$ and $E_1 \cap E_2 = \{uv\}$, say. Without loss of generality u has degree three in F_1. The fact that $\Delta \leq 3$, now tells us that u has degree one in F_2, which again gives a contradiction. Thus $F_1 \neq K_{2,3}$ and, by symmetry, $F_2 \neq K_{2,3}$.

Thus we must have $F_1 = H_4 = F_2$ and $|V_1 \cap V_2| \leq 5$. We first consider the case when $|V_1 \cap V_2| = 5$. Since $F_1 \cap F_2$ is a subgraph of F_1, $F_1 \cap F_2$ is either a path of length four, say $u_1u_2u_3u_4u_5$, or the graph obtained from a cycle of length four by adding a new vertex joined to exactly one vertex of the cycle. Since $F_1 = H_4 = F_2$, the former case would imply that u_3 has degree four in $F_1 \cup F_2$, and hence contradict $\Delta \leq 3$, whereas the latter case would imply that $F_1 \cup F_2$ can be obtained from a cycle of length six by adding a vertex joined to three vertices of the cycle, and hence contradict Claim 6.5(d). We next consider the case when $|V_1 \cap V_2| = 4$. Then $F_1 \cap F_2$ is either $K_{2,2}$, or $K_{1,3}$, or a path of length three, or two disjoint K_2's. If $F_1 \cap F_2 = K_{2,2}$ then $F_1 \cup F_2$ is a cycle of length eight with two long chords, contradicting Claim 6.5(c). If $F_1 \cap F_2 = K_{1,3}$ then the fact that $F_1 = F_2 = H_4$ implies that some vertex of $F_1 \cap F_2$ has degree at least four in $F_1 \cup F_2$ and contradicts $\Delta \leq 3$. If $F_1 \cap F_2$ is either a path of length three or two disjoint K_2's then $F_1 \cup F_2$ contains a cycle of length eight with two long chords, and hence contradicts Claim 6.5(c). We next consider the case when $|V_1 \cap V_2| = 3$. Then $F_1 \cap F_2$ is a path of length two, say $v_1v_2v_3$. Then v_1 and v_3 must have degree two in both F_1 and F_2. Since $\Delta \leq 3$, v_2 has degree two in either F_1 or F_2. This is impossible since neither F_1 nor F_2 contain three vertices of degree two which induce a path of length two. Finally, we consider the case when $|V_1 \cap V_2| = 2$. Then $F_1 \cap F_2$ is a path of length one, say uv. Then u and v must have degree two in both F_1 and F_2. Thus $F_1 \cup F_2$ contains a cycle of length eight with two long chords. This contradicts Claim 6.5(c) and completes the proof of the claim. •

For each pair of vertices $u, v \in V$, let $t_G(u,v)$ be the number of u,v-paths in G of length at most two. Let $G^{(2)}$ be the multigraph with vertex set V, in which each pair of vertices $u, v \in V$ is joined by $t_G(u,v)$ parallel edges. (Thus G^2 can be obtained from $G^{(2)}$ by replacing each set of parallel edges by a single edge.) Since each vertex $v \in V$, is the central vertex in $\binom{d(v)}{2}$ paths of length two, we have

$$|E(G^{(2)})| = \sum_{v \in V} \binom{d(v)}{2} + \frac{1}{2} \sum_{v \in V} d(v). \tag{8}$$

We next determine $|E(G^{(2)}) - E(G^2)|$. If $u, v \in V$ belong to a multiple edge in $G^{(2)}$ then u, v are either joined by a path of length one and a path of length two in G, or by two disjoint paths of length two in G. In the former case u, v belong to a triangle, that is to say a H_1-subgraph of G. In the latter case u, v belong to a a cycle of length four, that is to say a H_2-subgraph of G. Thus, in both cases, u, v belong to a special H_i subgraph of G, for some $1 \le i \le 4$. Since the special subgraphs of G are vertex disjoint by Claim 6.6, u, v belong to a unique special subgraph F. Thus we may determine $|E(G^{(2)}) - E(G^2)|$ by summing $|E(F^{(2)}) - E(F^2)|$ over all special subgraphs of G. Hence, if h_i is the number of special H_i-subgraphs of G, we have $|E(G^{(2)}) - E(G^2)| = 3h_1 + 2h_2 + 5h_3 + 4h_4$. Combining this with (8), and using n_j for the number of vertices of G of degree j, we obtain

$$|E(G^2)| = 2n_2 + \tfrac{9}{2}n_3 - 3h_1 - 2h_2 - 5h_3 - 4h_4. \tag{9}$$

Since G is superstrong, $5G - e$ has six edge-disjoint spanning trees for all $e \in E(5G)$. For each special subgraph F of G these trees can contain at most $5(|V(F)|-1)$ edges. Since the special subgraphs of G are vertex disjoint and each spanning tree has $|V|-1$ edges, we may deduce that

$$5|E| - 3h_1 - 2h_2 - 6h_3 - 5h_4 \ge 6|V| - 6, \tag{10}$$

with equality only if each edge $e \in E$ belongs to a special subgraph of G. Note that, since G is connected and the special subgraphs are vertex disjoint, this means that equality can occur only if G is the unique special subgraph of itself. Since $|V| = n_2 + n_3$ and $|E| = n_2 + \frac{3}{2}n_3$ we may use (10) to deduce that

$$\tfrac{3}{2}n_3 - n_2 \ge 3h_1 + 2h_2 + 6h_3 + 5h_4 - 6.$$

Using (9) we now obtain

$$\begin{aligned} |E(G^2)| &= 3n_2 + 3n_3 + \tfrac{3}{2}n_3 - n_2 - 3h_1 - 2h_2 - 5h_3 - 4h_4 \\ &\ge 3n_2 + 3n_3 - 6 = 3|V| - 6, \end{aligned}$$

with equality only if $h_3 = 0 = h_4$. Since equality can occur in (10) only if G is a special subgraph of itself, we deduce that $|E(G^2)| \ge 3|V| - 6$ with equality only if $|V| \le 4$. •

Lemma 6.7. *Let $G = (V, E)$ be a graph on at least three vertices such that G has maximum degree $\Delta \leq 3$, and each superbrick of G has at most four vertices. Then $|E(G^2)| \leq 3|V| - 6$.*

Proof: We proceed by induction on $|V| + |E|$. The lemma holds when $|V| = 3$ so we may suppose that $|V| \geq 4$. If G has a cycle of length four with a chord e then, since $\Delta \leq 3$, $(G-e)^2 = G^2$ and we are done by applying induction to $G - e$. Thus we may assume that no cycles of length four in G have chords. Suppose G has a vertex v with $d(v) \leq 1$. Then each superbrick of $G - v$ has size at most four and, since $\Delta \leq 3$, G^2 has at most three more edges than $(G-e)^2$. Thus we are done by applying induction to $G - v$. Hence we may assume that $d(v) \in \{2, 3\}$ for all $v \in V$. Let n_2, n_3 be the numbers of vertices of G of degree two and three, respectively, and put $|V| = n$.

Let $\mathcal{S}$ be the superbrick partition of G and let s_i be the number of superbricks in $\mathcal{S}$ with i vertices. (Thus $s_i = 0$ for $i \notin \{1, 3, 4\}$.) We have

$$0 \leq \mathrm{def}(G) = \mathrm{def}_G(\mathcal{S}) = 6(|\mathcal{S}| - 1) - 5e_G(\mathcal{S}). \tag{11}$$

Since $|E| = 3s_3 + 4s_4 + e_G(\mathcal{S})$ and $|\mathcal{S}| = s_1 + s_3 + s_4 = n - 2s_3 - 3s_4$, we may use (11) to obtain

$$|E| \leq 3s_3 + 4s_4 + \tfrac{6}{5}(n - 2s_3 - 3s_4 - 1) = \tfrac{1}{5}(6n + 3s_3 + 2s_4 - 6).$$

Since $n = n_2 + n_3$ and $|E| = n_2 + \frac{3}{2}n_3$, it follows that

$$\tfrac{3}{2}n_3 - n_2 \leq 3s_3 + 2s_4 - 6. \tag{12}$$

Since the superbricks of G are vertex disjoint, we may apply the argument used to deduce (9) to obtain

$$|E(G^2)| = 2n_2 + \tfrac{9}{2}n_3 - 3s_3 - 2s_4 = 3n_2 + 3n_3 + \tfrac{3}{2}n_3 - n_2 - 3s_3 - 2s_4. \tag{13}$$

Since $|V| = n_2 + n_3$, we may use (12) and (13) to deduce that $|E(G^2)| \leq 3|V| - 6$. •

Theorem 6.8. *Let G be a graph. Then G^2 is Laman if and only if each vertex of G has degree at most three and each superbrick of G has at most four vertices.*

Proof: First suppose that G^2 is Laman. Then G has maximum degree at most three by Lemma 6.2 and each superbrick of G has at most four vertices by Lemma 6.4.

Next suppose each vertex of G has degree at most three and each superbrick of G has at most four vertices. For a contradiction suppose that G^2 is not Laman and let X be a subset of $V(G)$ for which $h(X) = i_{G^2}(X) - (3|X| - 6)$ is as large as possible, and subject to this condition, $|X|$ is as large as possible. We have $h(X) \geq 1$ and $|X| \geq 3$. The maximality of $h(X)$ and $|X|$, and the fact that G has maximum degree at most three, imply that $G[X]$ has minimum degree at least one, and no vertex in $V - X$ is adjacent to two non-adjacent vertices of X in G. Thus $G^2[X] = G[X]^2$. Since $G[X]$ satisfies the hypotheses of Lemma 6.7, this implies $i_{G^2}(X) \leq 3|X| - 6$, a contradiction. •

Using Theorem 6.8 we may deduce that Conjecture 6.1 is equivalent to:

Conjecture 6.9. *Let G be a graph. Then G^2 is M-independent if and only if each vertex of G has degree at most three and each superbrick of G has at most four vertices.*

Conjecture 6.9 would imply that if G is a graph of maximum degree at most three and every superbrick of G has exactly one vertex, then G^2 is M-independent. By Lemmas 3.1(a) and 4.7 this is equivalent to:

Conjecture 6.10. *Let G be a graph of maximum degree at most three. If $5i(X) \leq 6(|X|-1)$ for all nonempty $X \subseteq V$, then G^2 is M-independent.*

We shall show in Section 8 below that Conjecture 6.10 is true under the stronger hypothesis that $10i(X) \leq 11(|X|-1)$ for all nonempty $X \subseteq V$.

Note that for graphs without cycles of length less than five, Conjectures 6.9 and 6.10 are equivalent. For this family of graphs these conjectures and Theorem 1.4(c) would imply:

Conjecture 6.11. *Let G be a graph without cycles of length three and four. Then G^2 is M-independent if and only if the edge set of $5G$ can be partitioned into six forests.*

7 Extending independent graphs

In this section we use Lemmas 2.1 and 2.2 to derive some more complex operations which preserve M-independence in a graph.

Lemma 7.1. *Let $H = (V, E)$ be an M-independent graph and $\{u_1, u_2, u_3\}$ and $\{v_1, v_2, v_3\}$ be two sets of distinct vertices of G (we allow the sets to have common vertices). Suppose $v_1v_2 \in E$. Let G be obtained from $H - v_1v_2$ by adding two new vertices u, v, the edge uv, and all edges uu_i, vv_i for $1 \leq i \leq 3$. Then G is M-independent.*

Proof: This follows from Lemmas 2.1 and 2.2, since G can be constructed from H by first performing a 0-extension with u, then a 1-extension with v. •

We refer to the operation in Lemma 7.1 as an *edge-extension*.

Lemma 7.2. *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 $|\{u_1, u_2, v_1, v_2, w_1, w_2\}| \geq 3$. 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 $1 \leq i \leq 2$. Then G is M-independent.*

Proof: By renaming the sets, if necessary, we may suppose that u_1, u_2, v_1 are distinct vertices. Then the lemma follows from Lemmas 2.1 and 7.1, since G can be constructed from H by first performing a 0-extension with u using u_1, u_2, v_1, then an edge-extension with v, w which deletes the edge uv_1. •

We refer to the operation in Lemma 7.2 as a *triangle-extension*.

Let G be a graph and u, v be, not necessarily distinct, vertices of G. A *uv-ear* in G is subgraph X which is a uv-path if $u \neq v$ or a cycle containing u if $u = v$, and is such that all vertices of $V(X) - \{u, v\}$ have degree two in G, and u, v both have degrees not equal to two in G. We say that X is an *ear of length* r if X has length r, and that X is a *closed ear* if X is a cycle.

The next two lemmas are due to Franzblau. We include proofs for the sake of completeness.

Lemma 7.3. *[3] Let $H = (V, E)$ be a graph such that H^2 is M-independent. Let G be obtained from H by attaching a uv-ear. Suppose u has degree three in G and v has degree one in G. Then G^2 is M-independent.*

Proof: We have $G = H \cup P$ where $P = ux_1x_2 \dots x_{r-1}v$ is an ear in G and $d_G(v) = 1$. We can construct G^2 from H^2 by a sequence of 0-extensions, we first add x_1, then x_2 and so on. Thus G^2 is M-independent by Lemma 2.1. •

Lemma 7.4. *[3] Let $H = (V, E)$ be a graph such that H^2 is M-independent. Let G be obtained from H by attaching a uv-ear of length at least six, where u, v both have degree three in G. (Note that $u = v$ may hold.) Then G^2 is M-independent.*

Proof: We have $G = H \cup X$ where $X = ux_1x_2 \dots x_{r-1}v$ is an ear in G of length $r \geq 6$. Let $F = H \cup (X - \{x_2, x_3, x_4\})$. Then F^2 is M-independent by two applications of Lemma 7.3. Since G^2 can be obtained from F^2 by a triangle-extension (using the triangle $x_2x_3x_4x_2$ of G^2), G^2 is M-independent by Lemma 7.2. •

Lemma 7.5. *Let $H = (V, E)$ be a graph. Let G be obtained from H by attaching a uv-ear of length at least five, where u, v both have degree three in G. If $H^2 + uv$ is M-independent, then G^2 is M-independent.*

Proof: We have $G = H \cup P$ where $P = ux_1x_2 \dots x_4v$ is an ear in G of length five. Since $F = G^2 - \{x_2, x_3\} + x_1x_4$ can be obtained from $H^2 + uv$ by two 1-extensions, it is M-independent by Lemma 2.2. Now G^2 can be obtained from F by an edge extension (adding the vertices x_2, x_3 and deleting the edge x_1x_4), so it is also M-independent by Lemma 7.1. •

A *claw of size* (r_1, r_2, r_3) attached at vertices v_1, v_2, v_3 in a graph G is a subgraph W of G which can be expressed as the union of three ears P_1, P_2, P_3 of G, where P_i is a v_iu-ear of length r_i for $1 \leq i \leq 3$ and u is a vertex of G of degree three. We will assume throughout that $r_1 \geq r_2 \geq r_3$.

Lemma 7.6. *Let $H = (V, E)$ be a graph such that H^2 is M-independent. Let G be obtained from H by attaching a claw W of size (r_1, r_2, r_3) at vertices v_1, v_2, v_3. Suppose v_1, v_2, v_3 all have degree three in G, $r_1 + r_2 + r_3 \geq 12$ and $r_2 + r_3 \geq 6$. Then G^2 is M-independent.*

Proof: We have $G = H \cup W$ and $W = P_1 \cup P_2 \cup P_3$ where P_i is a v_iu-ear in G of length r_i and $r_1 \geq r_2 \geq r_3$. Let $P_1 = v_1x_1x_2 \ldots x_{r_1-1}u$, $P_2 = v_2y_1y_2 \ldots y_{r_2-1}u$, and $P_3 = v_3z_1z_2 \ldots z_{r_3-1}u$.

We first consider the case when $r_1 \geq 6$. Let $F = H \cup P_2 \cup P_3$. Since H^2 is M-independent and $r_2 + r_3 \geq 6$, F^2 is M-independent by Lemma 7.4. Now, since $G = F \cup P_1$ and $r_1 \geq 6$, G^2 is M-independent, again by Lemma 7.4.

We next consider the case when $r_1 = r_2 = 5$. Since $r_1 + r_2 + r_3 \geq 12$, we have $r_3 \geq 2$. Let $F = H \cup (P_3 - u) \cup (P_2 - \{y_2, y_3, y_4, u\}$. Since H^2 is M-independent, F^2 is M-independent by Lemma 7.3. Let

$$G_1 = F^2 + u + \{uv_1, uz_{r_3-1}, uz_{r_3-2}\},$$

taking $z_{r_3-2} = v_3$ if $r = 2$. Then G_1 is a 0-extension of F^2 so is M-independent by Lemma 2.1. Let

$$G_2 = G_1 + \{y_2, y_3, y_4\} + \{y_2y_3, y_3y_4, y_4y_2, y_2v_2, y_2y_1, y_3y_1, y_3u, y_4u, y_4z_{r_3-1}\}.$$

Then G_2 is a triangle-extension of G_1 so is M-independent by Lemma 7.2. Since $G_2 = (H \cup P_2 \cup P_3)^2 + uv_1$, we can now apply Lemma 7.5 to deduce that G^2 is M-independent.

We next consider the case when $r_1 = 5$ and $r_2 = 4$. Since $r_1 + r_2 + r_3 \geq 12$, we have $r_3 \geq 3$. Let $F = H \cup (P_3 - \{u, z_{r_3-1}\}) \cup (P_2 - \{y_2, y_3, u\})$. Since H^2 is M-independent, F^2 is M-independent by Lemma 7.3. Let

$$G_1 = F^2 + \{u, z_{r_3-1}\} + \{uv_1, uy_1, uz_{r_3-2}, z_{r_3-1}u, z_{r_3-1}z_{r_3-2}, z_{r_3-1}z_{r_3-3}\},$$

taking $z_{r_3-3} = v_3$ if $r = 3$. Then G_1 can be obtained from F^2 by two 0-extensions, so is M-independent by Lemma 2.1. Let

$$G_2 = (G_1 - uy_1) + \{y_2, y_3\} + \{y_2y_3, y_2y_1, y_2v_2, y_2u, y_3y_1, y_3u, y_3z_{r_3-1}\}.$$

Then G_2 is an edge-extension of G_1 so is M-independent by Lemma 7.1. Since $G_2 = (H \cup P_2 \cup P_3)^2 + uv_1$, we can now apply Lemma 7.5 to deduce that G^2 is M-independent.

Finally we consider the case when $r_1 = r_2 = 4$. Since $r_1 + r_2 + r_3 \geq 12$ and $r_1 \geq r_2 \geq r_3$, we have $r_3 = 4$. Let $F = H \cup \{x_1, y_1, z_1\} \cup \{x_1v_1, y_1v_2, z_1v_3\}$. Since H^2 is M-independent, F^2 is M-independent by Lemma 7.3. Let $G_1 = F^2 + u + \{ux_1, uy_1, uz_1\}$. Then G_1 is a 0-extension of F^2, so is M-independent by Lemma 2.1. Let

$$G_2 = (G_1 - uy_1) + \{y_2, y_3\} + \{y_2y_3, y_2y_1, y_2v_2, y_2u, y_3y_1, y_3u, y_3x_1\}.$$

Then G_2 is an edge-extension of G_1 so is M-independent by Lemma 7.1. Let

$$G_3 = (G_2 - uz_1) + \{z_2, z_3\} + \{z_2z_3, z_2z_1, z_2z_{r_3-4}, z_2u, z_3u, z_3z_1, z_3y_3\}.$$

Then G_3 is an edge-extension of G_2 so is M-independent by Lemma 7.1. Let

$$G_4 = (G_3 - y_3x_1) + x_3 + \{x_3x_1, x_3u, x_3y_3, x_3z_3\}.$$

Then G_4 is a 1-extension of G_3 so is M-independent by Lemma 2.2. Finally, we have

$$G^2 = (G_4 - ux_1) + x_2 + \{x_2x_1, x_2x_3, x_2u, x_2v_1\}.$$

Thus G^2 is a 1-extension of G_4 so is M-independent by Lemma 2.2. •

8 Independent squares of sparse graphs

In this section we show that squares of sufficiently sparse graphs are M-independent.

Lemma 8.1. *Let $G = (V, E)$ be a connected graph in which all vertices have degree two or three. Suppose that G is not a cycle, G contains no closed ears, and $k|E| \leq (k+1)(|V|-1)$ for some positive integer k. Then G has a claw of size (r_1, r_2, r_3) for some $r_1 + r_2 + r_3 \geq k+2$.*

Proof: Let n_2, n_3 be the number of vertices of G of degree two and three respectively. Then $|E| = n_2 + \frac{3}{2}n_3$. Let H be the 3-regular multigraph obtained by suppressing all vertices of degree two in G and $w : E(H) \to \mathbb{Z}_+$ be defined by letting $w(e)$ be the length of the ear in G corresponding to e, for each $e \in E(H)$. Note that H is loopless since G has no closed ears. For $v \in V(H)$ let $w(v)$ be the sum of the weights of the edges incident to v. Then we have

$$\sum_{v \in V(H)} w(v) = 2|E| = 2n_2 + 3n_3. \tag{14}$$

Since $k|E| \leq (k+1)(|V|-1)$ we also have

$$k(n_2 + \tfrac{3}{2}n_3) \leq (k+1)(n_2 + n_3 - 1),$$

and hence $n_2 \geq \frac{1}{2}kn_3 - n_3 + k + 1$. Substituting into (14) we obtain

$$\sum_{v \in V(H)} w(v) \geq (k+1)n_3 + 2k + 2.$$

Thus there exists a vertex $v \in V(H)$ with $w(v) \geq k+2$. •

Theorem 8.2. *Let $G = (V, E)$ be a graph of maximum degree at most three. If $10i(X) \leq 11(|X|-1)$ for all nonempty $X \subseteq V$, then G^2 is M-independent.*

Proof: Suppose the theorem is false and choose a counterexample G with as few vertices as possible. Then G is connected. If G has a vertex v of degree one then we may choose a uv-ear P in G. Let $H = G - (P - u)$. By induction H^2 is M-independent. Thus G^2 is M-independent by Lemma 7.3. Hence all vertices of G have degree two or three.

Suppose G has a uv-ear P of length at least six, for some $u, v \in V$. Let $H = G - (P - \{u, v\})$. By induction H^2 is M-independent. Thus G^2 is M-independent by Lemma 7.4. Hence all ears of G have length at most five. Thus, since $10i(X) \leq 11(|X|-1)$ for all nonempty $X \subseteq V$, G is not a cycle and G contains no closed ears.

By Lemma 8.1, G has a claw W of size (r_1, r_2, r_3) where $r_1 + r_2 + r_3 \geq 12$. Since $r_1 < 6$, we have $r_2 + r_3 > 6$. Let v_1, v_2, v_3 be the vertices of attachment of W in G, and let $H = G - (W - \{v_1, v_2, v_3\})$. By induction H^2 is M-independent. Thus G^2 is M-independent by Lemma 7.6. •

9 Further remarks

In [9] we study the rigid components (i.e. maximal rigid subgraphs) of molecular graphs and show that two other conjectures in combinatorial rigidity (due to Dress and Jacobs, respectively) imply Conjecture 1.3. Furthermore, by assuming the truth of Conjecture 1.2, we give an efficient algorithm for computing the rigid components of a molecular graph.

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