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Highly connected molecular graphs are rigid in three dimensions

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Abstract

We show that every 7-vertex-connected molecular graph is generically rigid in three dimensions. This verifies a special case of a conjecture of Lovász and Yemini. For this family of graphs the bound is best possible.

1 Introduction

Lovász and Yemini [6] conjectured in 1982 that there exists a constant c such that every c-vertex-connected graph is rigid in three-space, when it is realized as a generic bar-and-joint framework. Their conjecture is still open. The existence of 11-vertex-connected non-rigid graphs shows that if c exists, it is at least 12. Note that the characterization of rigid graphs in three-space is a difficult unsolved problem. The reader is referred to [1, 11] for basic definitions and results of combinatorial rigidity.

In this paper we consider an important special case, which has been a focus of recent research: squares of graphs. The *square* G^2 of a graph G is obtained from G by adding a new edge uv for each pair $u, v \in V(G)$ of distance two in G, see Figure 1. Squares of graphs are sometimes called *molecular graphs*, because they are used to study the flexibility of molecules [2, 10, 12].

We shall verify the conjecture of Lovász and Yemini in the special case of molecular graphs by showing that every 7-vertex-connected molecular graph is rigid in three dimensions. We also give an example showing that for this family of graphs the bound is best possible.

Our proof relies on a recent result of Katoh and Tanigawa [5], who characterized rigid molecular graphs in three-space[1]. For a graph G let $5G$ denote the multigraph obtained from G by replacing each edge $e \in E(G)$ by five copies of e.

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[1]Katoh and Tanigawa [5] proved the Molecular Conjecture due to Tay and Whiteley [8, Conjecture 1], which is formulated in terms of non-generic d-dimensional body-and-hinge frameworks, for $d \geq 2$. The bar-and-joint version, given in Theorem 1.1, can be deduced from the three-dimensional version of their result, see e.g. [3]. Note that a direct proof for the necessity of the spanning tree condition and an extension of Theorem 1.1, characterizing the degrees of freedom of a molecular graph, can be found in [3].

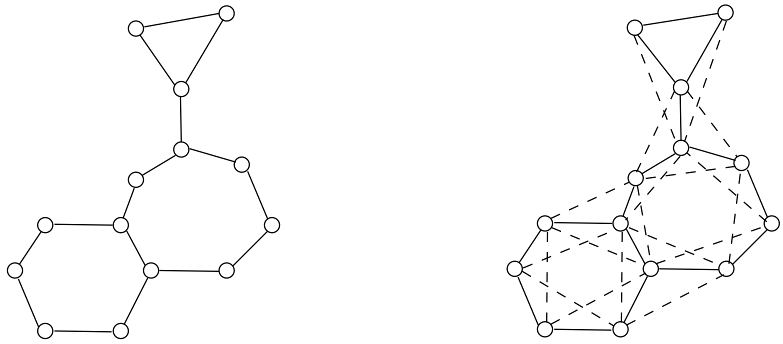

Figure 1: A graph G and its square G^2, obtained from G by adding the dashed edges.

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

Let $G = (V, E)$ be a graph. For a partition $\mathcal{P}$ of V let $e_G(\mathcal{P})$ denote the number of edges of G connecting distinct members of $\mathcal{P}$. Let

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

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

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

We say that a partition $\mathcal{P}$ of V is a *tight partition of* G if $\text{def}_G(\mathcal{P}) = \text{def}(G)$. Note that $\text{def}(G) \geq 0$ since $\text{def}_G(\{V\}) = 0$. By a celebrated result of Tutte and Nash-Williams $5G$ contains six edge-disjoint spanning trees if and only if $\text{def}(G) = 0$. We shall use this fact and deficient partitions in the next section.

2 Highly connected molecular graphs

Let $G = (V, E)$ be a graph. For a subset $U \subseteq V$ let $\delta(U)$ denote the set of edges connecting U and $V - U$. A subset F of E is called an *edge-cut* if $F = \delta(U)$ for some $U \subseteq V$. A subset U of V is called a *vertex-cut* if $G - U$ is disconnected. G is said to be *k-vertex-connected* if $|V| \geq k + 1$ and there is no vertex-cut in G containing less than k vertices. Let $F = \delta(U)$ be an edge-cut. The *border* of F, denoted $B(F)$, is the set of end-vertices of the edges of F. We say that F is *essential* if $U - B(F)$ and $V - U - B(F)$ are both non-empty.

Proposition 2.1. *Suppose that G has an essential edge-cut of size f. Then G^2 has a vertex-cut of size at most $2f$.*

Proof: Let F be an essential edge-cut in G. Then $G^2 - B(F)$ is disconnected. Since $|B(F)| \leq 2|F|$, the proposition follows. •

Our goal is to prove that if G^2 is not rigid then G has an essential edge-cut of size at most three. First we need a lemma about 'claws'.

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.

Let v be a vertex of degree i, $i \geq 3$, which is not incident with any closed ears. Then the *i-claw centered at* v is the subgraph of G which is the union of the i ears $P_1, P_2, ..., P_i$ incident with v. We say that the claw is of *size* $(r_1, r_2, ..., r_i)$, where ear P_j is of length r_j, $1 \leq j \leq i$. We will assume throughout that $r_1 \geq r_2 \geq ... \geq r_i$.

Lemma 2.2. *Let $G = (V, E)$ be a connected graph with minimum degree at least two. Suppose that G is not a cycle, G contains no closed ears, and $5|E| \leq 6(|V| - 1)$. Then G has an i-claw of size $(r_1, r_2, ..., r_i)$ with $\sum_1^i r_j \geq 6(i-2)+1$ for some $i \geq 3$.*

Proof: Let H be the 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 is not a cycle and G contains no closed ears, and H has minimum degree at least three.

For $v \in V(H)$ let $w(v)$ be the sum of the weights of the edges incident to v and let n_i be the number of vertices of degree i in G, $i \geq 2$. Then we have

$$\sum_{v \in V(H)} w(v) = 2|E| = \sum_{i=2}^{\Delta(G)} i n_i, \tag{1}$$

where $\Delta(G)$ denotes the maximum degree in G. Since $5|E| \leq 6(|V| - 1)$, we also have

$$5\Big(\sum_{i=2}^{\Delta(G)} \frac{i}{2} n_i\Big) \leq 6\Big(\sum_{i=2}^{\Delta(G)} n_i\Big) - 6, \tag{2}$$

and hence

$$n_2 \geq \sum_{i=3}^{\Delta(G)} \frac{5i-12}{2} n_i + 6. \tag{3}$$

Substituting into (1) we obtain

$$\sum_{v \in V(H)} w(v) \geq \sum_{i=3}^{\Delta(G)} (5i-12)n_i + i n_i + 12 = \sum_{i=3}^{\Delta(G)} 6(i-2)n_i + 12. \tag{4}$$

Thus there exists a vertex $v \in V(H)$ with $d(v) = i$ and $w(v) \geq 6(i-2)+1$, for some $i \geq 3$. •

Let $G = (V, E)$ be a graph and $X \subseteq V$. We use $i_G(X)$ to denote the number of edges induced by X in G.

Lemma 2.3. *Let G be a graph with minimum degree at least two. Suppose that*

$$5i_G(X) < 6(|X| - 1) \tag{5}$$

for all $X \subseteq V$ with $|X| \geq 2$. Then G has an essential edge-cut of size at most three.

Proof: Observe that (5) implies that G has no cycles of length at most six. First suppose that G is a cycle or G contains a closed ear. Then the cycle (or the closed ear) must have length at least seven, which implies that there is an essential edge-cut in G of size at most two. Thus we may suppose that G is not a cycle and G contains no closed ears.

Consider an i-claw of size $(r_1, r_2, ..., r_i)$ with $\sum_1^i r_j \geq 6(i-2)+1$ with center v, which exists by Lemma 2.2.

First suppose $i \geq 4$. Then $6(i-2)+1 \geq 3i+1$, which implies $r_1 \geq 4$. Let $vx_1x_2...x_{r-1}u$ be the sequence of vertices of P_1. Put $U = \{x_1, x_2, ..., x_{r-1}\}$. We claim that $F = \delta(U)$ is an essential edge-cut. It is clear that $x_2 \in U - B(F)$. If $r_2 \geq 2$ then any inner vertex of P_2 is in $V - U - B(F)$. If $r_2 = 1$ then, since $i (\geq 4) \geq 3$ and G is simple, P_2 or P_3 must have an end-vertex which is different from v and also different from u. This vertex is in $V - U - B(F)$. Thus F is essential. Since F has size two, the lemma follows when $i \geq 4$.

Next suppose $i = 3$. Then $r_1 + r_2 + r_3 \geq 7$. If $r_1 \geq 4$ then we are done as above, so we may assume that $r_1 = 3$. Let P_1, P_2, P_3 be the ears incident with v with end-vertices u_1, u_2, u_3. Since G has no cycles of length at most six, we can deduce that u_1, u_2, u_3 are pairwise distinct.

Let $U = \{v, x_1, x_2\}$, where x_1, x_2 are the inner vertices of P_1. Then $F = \delta(U)$ is an essential edge-cut. This follows by observing that $x_1 \in U - B(F)$ and $u_2 \in V - U - B(F)$. We have $|F| \leq 3$. This completes the proof of the lemma. •

We can now prove our main result. Let $G = (V, E)$ be a connected graph on at least two vertices. 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 the minimum degree of G is at least two.

Theorem 2.4. *Let G be a graph and suppose that G^2 is 7-connected. Then G^2 is rigid in three-space.*

Proof: First suppose that G_{core} is empty, which is equivalent to saying that G is a tree. In this case it is easy to see that either G has an essential edge-cut F of size one, or G is a star. In the former case G^2 cannot be 7-connected by Proposition 2.1, a contradiction. In the latter case G^2 is a complete graph, which is rigid, as required.

Thus we may assume that G_{core} is non-empty. As above, it is easy to see that if G has a vertex v of degree at least two which does not belong to the core then G has an essential edge-cut F of size one, a contradiction by Proposition 2.1. It follows that each vertex not in the core of G has degree one. In this case G^2 is rigid if G^2_{core} is rigid (which is easy to see, see e.g. [3, Lemma 4.2]). Hence it suffices to prove that G^2_{core} is rigid.

Let $H = G_{core}$ and suppose, for a contradiction, that H^2 is not rigid. Then it follows from Theorem 1.1 that $\mathrm{def}(H) \geq 1$. Consider a tight partition $\mathcal{P} = \{X_1, X_2, ..., X_t\}$ of H for which $|\mathcal{P}|$ is as small as possible. Let $K = (W, F)$ denote the graph obtained from H by contracting each member X_i to a single vertex x_i, $1 \leq i \leq t$. By the choice of $\mathcal{P}$ we must have

$$5i_K(X) < 6(|X| - 1) \tag{6}$$

for all $X \subseteq W$ with $|X| \geq 2$ (see [4, Lemma 2.2(b)]).

We can now use Lemma 2.3 to deduce that K has an essential edge-cut of size at most three. Thus H also has an essential edge-cut of size at most three, which is an essential edge-cut in G, too. Thus, by Proposition 2.1, G^2 is not 7-connected. This contradiction completes the proof of the theorem. •

The graph in Figure 2 shows that the bound on the vertex-connectivity of G^2 is best possible.

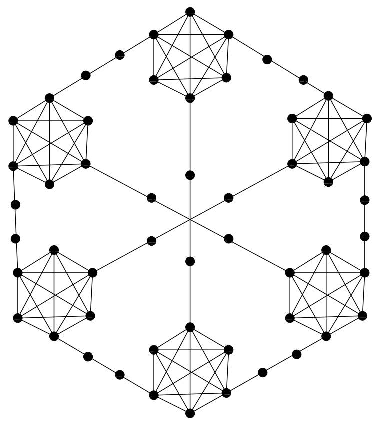

Figure 2: The square of this graph G is 6-connected and non-rigid. To see that G^2 is not rigid consider the partition $\mathcal{P}$ of $V(G)$ consisting of the vertex sets of the six copies of K_6 and the remaining eighteen copies of K_1. Since $\mathrm{def}(G) \geq \mathrm{def}_G(\mathcal{P}) = 3 > 0$, $5G$ does not contain six edge-disjoint spanning trees, and hence G^2 is not rigid by Theorem 1.1.

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