分子構造に関する剛性予想の証明

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概要　d 次元空間上の剛体ヒンジ構造とは d 次元の部分空間 (剛体) が $(d-2)$ 次元アフィン空間 (ヒンジ) によって接続された構造物であり，各剛体は接続されたヒンジ周りを回転し動く事が出来る．特に各剛体が $(d-1)$ 次元アフィン空間 (剛板) として実現される際，構造物は剛板ヒンジ構造と呼ばれる．剛体ヒンジ構造物の 1 次剛性は，その接続関係の組合せ構造によって特徴付けされる事が知られており，1984 年に Tay and Whiteley はその組合せ的特徴付けが剛板ヒンジ構造物に対しても適用可能であると予想した．より正確には「グラフ G に対して，各頂点を剛板，各辺をヒンジに対応させ実現される剛板ヒンジ構造が全体として剛となる必要十分条件は $\left(\binom{d+1}{2}-1\right)G$ が $\binom{d+1}{2}$ 個の辺素な全域木を含む事である」という予想を彼らは行った．ここで $\left(\binom{d+1}{2}-1\right)G$ は G の各辺を $\left(\binom{d+1}{2}-1\right)$ 個の多重辺で置き換えたグラフである．3 次元空間において分子構造の 1 次剛性は剛板ヒンジ構造物を用いて表現できる事が知られており，そのためこの予想は “the Molecular Conjecture” と呼ばれている．本稿では，長年未解決であったこの予想に対する証明を与える．またこの結果から，G^2 の辺集合を台集合とする 3 次元剛性マトロイドの組合せ的特徴付けが得られる．

A Proof of the Molecular Conjecture

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Abstract　A d-dimensional body-and-hinge framework is, roughly speaking, a structure consisting of rigid bodies connected by hinges in d-dimensional space. The generic infinitesimal rigidity of a body-and-hinge framework has been characterized in terms of the underlying multigraph independently by Tay and Whiteley as follows: A multigraph G can be realized as an infinitesimally rigid body-and-hinge framework by mapping each vertex to a body and each edge to a hinge if and only if $\left(\binom{d+1}{2}-1\right)G$ contains $\binom{d+1}{2}$ edge-disjoint spanning trees, where $\left(\binom{d+1}{2}-1\right)G$ is the graph obtained from G by replacing each edge by $\left(\binom{d+1}{2}-1\right)$ parallel edges. In 1984 they jointly posed a question about whether their combinatorial characterization can be further applied to a nongeneric case. Specifically, they conjectured that G can be realized as an infinitesimally rigid body-and-hinge framework if and only if G can be realized as that with the additional “hinge-coplanar” property, i.e., all the hinges incident to each body are contained in a common hyperplane. This conjecture is called the Molecular Conjecture due to the equivalence between the infinitesimal rigidity of “hinge-coplanar” body-and-hinge frameworks and that of bar-and-joint frameworks derived from molecules in 3-dimension. In 2-dimensional case this conjecture has been proved by Jackson and Jordán in 2006. In this paper we prove this long standing conjecture affirmatively for general dimension. Also, as a corollary, we obtain a combinatorial characterization of the 3-dimensional bar-and-joint rigidity matroid of the square of a graph.

1 Introduction

A d-dimensional *body-and-hinge framework* is, roughly speaking, the collection of d-dimensional *rigid bodies* connected by *hinges*, where a hinge is a $(d-2)$-dimensional affine subspace, i.e. pin-joints in 2-space and line-hinges in 3-space and etc. The bodies are allowed to move continuously in $\mathbb{R}^d$ so that the relative motion of any two bodies connected by a hinge is a rotation around it and the framework is called *rigid* if every such a motion provides a framework isometric to the original one. The infinitesimal rigidity of this physical model can be formulated in terms of a linear homogeneous system by using the fact that any continuous rotation of a point around a $(d-2)$-dimensional affine subspace or any transformation to a fixed direction can be described by a $\binom{d+1}{2}$-dimensional vector, so-called a *screw center*. The formal definition will be given in the next section.

Let $G=(V,E)$ be a *multigraph* which may contain multiple edges. We consider a body-and-hinge framework as a pair $(G,\mathbf{q})$ where $\mathbf{q}$ is a mapping from $e\in E$ to a $(d-2)$-dimensional affine subspace $\mathbf{q}(e)$ in $\mathbb{R}^d$, i.e., $v\in V$ corresponds to a body and $uv\in E$ corresponds to a hinge $\mathbf{q}(uv)$ which joins two bodies associated with u and v. The framework $(G,\mathbf{q})$ is called a *body-and-hinge realization* of G.

We assume that the dimension d is a fixed integer with $d\geq 2$ and we shall use the notation D to denote $\binom{d+1}{2}$. For a multigraph $G=(V,E)$ and a positive integer k, the graph obtained by replacing each edge by k parallel edges is denoted by kG. In this paper, for our special interest in $(D-1)G$, we shall use the simple notation $\widetilde{G}$ to denote $(D-1)G$ and let $\widetilde{E}$ be the edge set of $\widetilde{G}$. Tay [12] and Whiteley [17] independently proved that the generic infinitesimal rigidity of a body-and-hinge framework is determined by the underlying (multi)graph as follows.

Proposition 1.1. ([12, 17]) *A multigraph G can be realized as an infinitesimally rigid body-and-hinge framework in $\mathbb{R}^d$ if and only if $\widetilde{G}$ has D edge-disjoint spanning trees.*

A body-and-hinge framework $(G, \mathbf{q})$ is called *coplanar* if, for each $v \in V$, all of the $(d-2)$-dimensional affine subspaces $\mathbf{q}(e)$ for the edges e incident to v are contained in a common $(d-1)$-dimensional affine subspace (i.e. a hyperplane). Following a clear physical interpretation, we shall refer to a coplanar body-and-hinge framework as a *panel-and-hinge framework* throughout the paper, i.e., each body is regarded as a panel ($(d-1)$-dimensional affine subspace) in $\mathbb{R}^d$. In 1984, Tay and Whiteley [13] jointly posed the following conjecture.

Conjecture 1.2. ([13]) *Let $G = (V, E)$ be a multigraph. Then, G can be realized as an infinitesimally rigid body-and-hinge framework in $\mathbb{R}^d$ if and only if G can be realized as an infinitesimally rigid panel-and-hinge framework in $\mathbb{R}^d$.*

Conjecture 1.2 is known as the *Molecular Conjecture* which has appeared in several different forms [16, 19] and has been a long standing open problem in the rigidity theory. For the special case when $d = 2$, Whiteley [18] proved affirmatively for the special class of multigraphs in 1989 and recently the conjecture has been completely proved by Jackson and Jordán [6]. The idea of their proof is to replace each body of a panel-and-hinge framework by a rigid bar-and-joint framework (called a rigid component) and reduce the problem to that for bar-and-joint frameworks. The definition of a bar-and-joint framework can be found in e.g. [19]. By using well-investigated properties of 2-dimensional bar-and-joint frameworks, they successfully proved the conjecture. Also, Jackson and Jordán [8] showed the *sufficient* condition for higher dimension; G has a panel-and-hinge realization in $\mathbb{R}^d$ if $(d-1)G$ has d edge-disjoint spanning trees.

In this paper we settled the Molecular Conjecture affirmatively in general dimension. Although the story-line of our proof is slightly close to that of [6] for 2-dimension, we remark that our proof directly provides a construction of an infinitesimally rigid panel-and-hinge framework, which is a main (and huge) difference from [6].

In $\mathbb{R}^3$ the rigidity of panel-and-hinge frameworks have a special relation with the flexibility of molecules. A molecular structure can be modeled as a body-and-hinge framework by representing atoms (vertices) as rigid bodies and bonds (edges) as hinges in such a way that all the hinges (lines) incident to each body are intersecting each other at the center of the body (with small adjustments, see e.g. [20, page 122]). Such a body-and-hinge framework is called *hinge-concurrent*. Since taking projective dual in $\mathbb{R}^3$ transforms points to planes, lines to lines and planes to points preserving their incidences, a hinge-concurrent body-and-hinge framework is mapped to a panel-and-hinge framework. Crapo and Whiteley [2] showed that taking the projective dual preserves the rigidity, which implies that G has an infinitesimally rigid hinge-concurrent body-and-hinge realization if and only if it has an infinitesimally rigid panel-and-hinge realization.

Another framework which models the flexibility of a molecule is a bar-and-joint framework of the *square* of a graph (see e.g. [5, 14, 20]). The square of a graph $G = (V, E)$ is defined as $G^2 = (V, E^2)$, where $E^2 = E \cup \{uv \in V \times V \mid u \neq v \text{ and } uw, wv \in E \text{ for some } w \in V \setminus \{u, v\}\}$. For a graph G of minimum degree at least two it is known that a bar-and-joint framework of G^2 is equivalent to a hinge-concurrent body-and-hinge framework of G in terms of the infinitesimal rigidity in $\mathbb{R}^3$ [5]. Combining this previous result with our proof of the Molecular Conjecture, we obtain a combinatorial characterization of the 3-dimensional rigidity of the square of a graph.

The paper consists of six sections. In Section 2 we shall provide a formal definition of the infinitesimal rigidity of body-and-hinge frameworks. In Section 3 we will provide several preliminary results concerning edge-disjoint spanning trees. In Sections 4 and 5 we will investigate combinatorial properties of multigraphs G such that $\widetilde{G}$ contains D edge-disjoint spanning trees. Such graphs are called *body-and-hinge rigid graphs* and edge-inclusionwise minimal graphs are called *minimally body-and-hinge rigid graphs* throughout the paper. In particular, in Section 5, we will show that any minimally body-and-hinge rigid graph can be reduced to a smaller minimally body-and-hinge rigid graph by the contraction of a proper rigid subgraph or a splitting off operation (defined in Section 5) at a vertex of degree two. Finally, in Section 6, we will provide a proof of the Molecular Conjecture by showing that any minimally body-and-hinge rigid graph G has a rigid panel-and-hinge realization. The proof is done by induction on the graph size. More precisely, following the construction of a graph given in Section 5, we convert G to a smaller minimally body-and-hinge rigid graph G'. From the induction hypothesis there exists a rigid panel-and-hinge realization of G'. We will show that we can extend this realization to that of G with a slight modification so that the resulting framework becomes rigid.

2 Body-and-hinge Frameworks

In this section we shall provide a formal definition of body-and-hinge frameworks. Please refer to [2, 8, 15] for more detailed descriptions.

Infinitesimal motions of a rigid body. A *body* in $\mathbb{R}^d$ is a set of points which affinely spans $\mathbb{R}^d$. An *infinitesimal motion* of a body is an isometric linear transformation of the body, i.e., the distance between any two points in the body are preserved after the transformation. It is known that the set of infinitesimal motions of a body forms a D-dimensional vector space, i.e., an infinitesimal motion is a linear combination of d translations and $\binom{d}{d-2}$ rotations around $(d-2)$-affine subspaces. Throughout the paper, we use the notation $\langle S \rangle$ to denote the linear subspace of $\mathbb{R}^d$ spanned by $S \subseteq \mathbb{R}^d$.

Let us review how to describe an infinitesimal rotation of a body around a $(d-2)$-affine subspace A in $\mathbb{R}^d$. Let $\boldsymbol{p}_1, \ldots, \boldsymbol{p}_{d-1}$ be $d-1$ points in $\mathbb{R}^d$ which affinely span A. Let M_A be the $(d-1) \times (d+1)$-matrix whose i-th row vector is the projective point $(\boldsymbol{p}_i, 1)$ in projective $(d+1)$-space. Let $s_{i,j}(A) = (-1)^{i+j-1} \det M_A^{i,j}$ with $1 \le i < j \le d+1$, where $M_A^{i,j}$ is the $(d-1) \times (d-1)$-submatrix of M_A obtained by deleting the i-th and j-th columns of M_A. Consider the D-dimensional vector $S(A) = (s_{i,j}(A))$ whose components $s_{i,j}(A)$ are arranged in the lexicographical ordering of the pair (i, j). A vector in $\langle S(A) \rangle$ is called a *screw center* of A.

For a point $\boldsymbol{q} \in \mathbb{R}^d$, let $M_{A,\boldsymbol{q}}$ be the $d \times (d+1)$-matrix obtained from M_A by adding $(\boldsymbol{q}, 1)$ as a new row. Let $\boldsymbol{v}_{A,\boldsymbol{q}} = (v_i)$ be the vector of length $d+1$ whose i-th component is defined by $v_i = (-1)^i \det M_{A,\boldsymbol{q}}^i$ for $1 \le i \le d+1$, where $M_{A,\boldsymbol{q}}^i$ is the submatrix obtained by deleting the i-th column of $M_{A,\boldsymbol{q}}$. Note that, denoting j-th component of $\boldsymbol{q}$ by q_j and letting $q_{d+1} = 1$, we have $v_i = \sum_{1 \le j \le d+1, j \ne i} q_j s_{i,j}(A)$. This implies that $\boldsymbol{v}_{A,\boldsymbol{q}}$ can be expressed by $\boldsymbol{v}_{A,\boldsymbol{q}} = M(\boldsymbol{q}\ 1)^\top$ with some $(d+1) \times (d+1)$-matrix M determined by $S(A)$. Such a calculation is conventionally denoted by $\boldsymbol{v}_{A,\boldsymbol{q}} = S(A) \vee \boldsymbol{q}$. An elementary geometric argument tells us that the d-dimensional vector $(v_1, v_2, \ldots, v_d)$ consisting of the first d components of $\boldsymbol{v}_{A,\boldsymbol{q}}$ is proportional to the instantaneous velocity at $\boldsymbol{q}$ induced by a rotation around A.

Although the details are omitted, it is known that an infinitesimal translation of a rigid body in the direction of a vector $\boldsymbol{x} \in \mathbb{R}^d$ is also described in terms of a screw center $S(\boldsymbol{x})$ (that is, a D-dimensional vector) by taking $d-1$ projective points at infinity. Namely, the first d components of $S(\boldsymbol{x}) \vee \boldsymbol{q}$ represents the infinitesimal translation at $\boldsymbol{q}$ to the direction $\boldsymbol{x}$.

An arbitrary infinitesimal motion of a body B can expressed in terms of screw centers as follows. An infinitesimal motion for a body is a linear combination of rotations and translations. Let $S_1, S_2, \ldots, S_D$ be the screw centers corresponding to these rotations and translations. Then, a *screw center* S for an arbitrary infinitesimal motion can be written as $S = \sum_{i=1}^{D} S_i$. The infinitesimal velocity at $\boldsymbol{q} \in B$ is thus calculated by taking the first d components of the $(d+1)$-dimensional vector $S \vee \boldsymbol{q}$.

Body-and-hinge frameworks. Suppose two bodies B and B' are joined to a hinge, which is a $(d-2)$-affine subspace A of $\mathbb{R}^d$. Let S and S' be screw centers of infinitesimal motions applied to B and B', respectively. Then, the hinge constraint, which imposes a relative motion of B and B' to be a rotation about A, can be described by $S - S' \in \langle S(A) \rangle$.

A *d-dimensional body-and-hinge framework* $(G, \mathbf{p})$ is a multigraph $G = (V, E)$ with a map $\mathbf{p}$ which associates a $(d-2)$-affine subspace $\mathbf{p}(e)$ of $\mathbb{R}^d$ with each $e \in E$. An *infinitesimal motion* of $(G, \mathbf{p})$ is a map $S : V \to \mathbb{R}^D$ such that $S(u) - S(v) \in \langle S(\mathbf{p}(e)) \rangle$ for every $e = uv \in E$. Namely, S is an assignment of a screw center $S(u)$ to the body of $u \in V$. An infinitesimal motion S is called *trivial* if $S(u) = S(v)$ for all $u, v \in V$ and we say that $(G, \mathbf{p})$ is *infinitesimal rigid* if all infinitesimal motions of $(G, \mathbf{p})$ are trivial.

Rigidity matrix. Let us introduce the matrix whose null space is the set of infinitesimal motions of $(G, \mathbf{p})$. We have defined that S is an infinitesimal motion of $(G, \mathbf{p})$ if and only if $S(u) - S(v) \in \langle S(\mathbf{p}(e)) \rangle$ for all $e = uv \in E$. Thus, taking any basis $\{r_1(\mathbf{p}(e)), r_2(\mathbf{p}(e)), \ldots, r_{D-1}(\mathbf{p}(e))\}$ of the orthogonal complement of $\langle S(\mathbf{p}(e)) \rangle$, we can say that S is an infinitesimal motion of $(G, \mathbf{p})$ if and only if $(S(u) - S(v)) \cdot r_i(\mathbf{p}(e)) = 0$ for $1 \le i \le D-1$ and $e = uv \in E$. Hence, the constraints to be an infinitesimal motion are described by $(D-1)|E|$ linear equations over $S(v) \in \mathbb{R}^D$ for $v \in V$. Consequently, we obtain $(D-1)|E| \times D|V|$-matrix $R(G, \mathbf{p})$ associated with this homogeneous system of linear equations such that sequences of consecutive $(D-1)$ rows are indexed by the elements of E and sequences of consecutive D columns are indexed by the elements of V. To describe it more precisely, let us denote by $R(\mathbf{p}(e))$ the $(D-1) \times D$-matrix whose i-th row vector is $r_i(\mathbf{p}(e))$. Then, the submatrix $R_{G,\mathbf{p}}[e, w]$ of $R(G, \mathbf{p})$ induced by the consecutive $(D-1)$ rows indexed by $e = uv \in E$ and the consecutive D columns indexed by $w \in V$ is written as $R_{G,\mathbf{p}}[e, w] = R(\mathbf{p}(e))$ if $w = u$, $R_{G,\mathbf{p}}[e, w] = -R(\mathbf{p}(e))$ if $w = v$ and otherwise $R_{G,\mathbf{p}}[e, w] = \mathbf{0}$. We call $R(G, \mathbf{p})$ the *rigidity matrix* of $(G, \mathbf{p})$ (see Fig. 1).

The null space of $R(G, \mathbf{p})$ is the space of all infinitesimal motions. We remark that the dimension of the null space, or equivalently that of the space of all infinitesimal motions, is uniquely determined by $(G, \mathbf{p})$ although the entries of $R(G, \mathbf{p})$ may vary depending on the choice of basis of the orthogonal

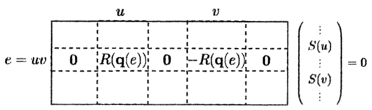

Figure 1: The rigidity matrix.

complement of $\langle S(\mathbf{p}(e))\rangle$.

It is not difficult to check that $(G, \mathbf{p})$ is infinitesimally rigid if and only if the rank of $R(G, \mathbf{p})$ is exactly $D(|V|-1)$. The dimension of the space of nontrivial infinitesimal motions is called the *degree of freedoms* of $(G, \mathbf{p})$, which is equal to $D(|V|-1) - \operatorname{rank} R(G, \mathbf{p})$. A body-and-hinge framework $(G, \mathbf{p})$ is called *generic* if the degree of freedoms is minimum or equivalently the rank of $R(G, \mathbf{p})$ is maximum taken over all realizations of G.

3 Edge-disjoint Spanning Trees

We use the following notations throughout the paper. Let $G = (V, E)$ be a multigraph. For $X \subseteq V$, let $G[X]$ be the graph induced by X. For $F \subseteq E$, let $V(F)$ be the vertices spanned by F, i.e., $V(F) = \{v \in V \mid uv \in F\}$, and let $G[F]$ be the graph edge-induced by F, i.e., $G[F] = (V(F), F)$. For $X \subseteq V$, let $\delta_G(X) = \{uv \in E \mid u \in X, v \notin X\}$ and let $d_G(X) = |\delta_G(X)|$. We shall omit set brackets when describing singleton sets, e.g., $d_G(v)$ implies $d_G(\{v\})$. For a partition $\mathcal{P}$ of V, let $d_G(\mathcal{P})$ denote the number of edges of G connecting distinct subsets of $\mathcal{P}$, respectively.

We use the following conventional notation. For a partition $\mathcal{P}$ of V, the *c-deficiency* of $\mathcal{P}$ in G is defined by $\operatorname{def}_{c,G}(\mathcal{P}) = c(|\mathcal{P}|-1) - d_G(\mathcal{P})$, and the *c-deficiency* of G is defined by $\operatorname{def}_c(G) = \max\{\operatorname{def}_{c,G}(\mathcal{P}) : \mathcal{P} \text{ is a partition of } V\}$. Note that $\operatorname{def}_c(G) \geq 0$ since $\operatorname{def}_{c,G}(\{V\}) = 0$. The Tutte-Nash-Williams tree packing theorem [10, 21] implies that G has d edge-disjoint spanning trees if and only if $\operatorname{def}_c(G) = 0$.

There is the other well-known characterization of an edge set containing c edge-disjoint spanning trees, which is written in terms of a *matroid* (see e.g. [11] for the definition and fundamental results of a matroid). For a multigraph $G = (V, E)$, let us consider the matroid on E, denoted by $\mathcal{M}_c(G)$, induced by the following nondecreasing submodular function $f_c : 2^E \to \mathbb{Z}$; for any $F \subseteq E$, $f_c(F) = c(|V(F)|-1)$. Namely, $F \subseteq E$ is *independent* in $\mathcal{M}_c(G)$ if and only if $|F'| \leq f_c(F')$ holds for every nonempty $F' \subseteq F$ (c.f. [11, Chapter 12]). It is known that G contains c edge-disjoint spanning trees if and only if the rank of $\mathcal{M}_c(G)$ is equal to $c(|V|-1)$.

Proposition 1.1 now implies that G can be realized as an infinitesimal rigid body-and-hinge framework if and only if the rank of $\mathcal{M}_D(\widetilde{G})$ is equal to $D(|V|-1)$. We shall simply denote $\mathcal{M}_D$ by $\mathcal{M}$. A more detailed relation between the deficiency of a graph and the rank of the rigidity matrix can be found in [8]. Let us summarize these preliminary results.

Proposition 3.1. ([8, 12, 17]) *The followings are equivalent for a multigraph $G = (V, E)$:*

(a) A generic body-and-hinge framework $(G, \mathbf{p})$ has k degree of freedoms.
(b) A generic body-and-hinge framework $(G, \mathbf{p})$ satisfies $\operatorname{rank} R(G, \mathbf{p}) = D(|V|-1) - k$.
(c) $\operatorname{def}_D(\widetilde{G}) = k$.
(d) The rank of $\mathcal{M}(\widetilde{G})$ is equal to $D(|V|-1) - k$.

4 Body-and-hinge Rigid Graphs

In this section we shall further investigate combinatorial properties of body-and-hinge frameworks. Let $G = (V, E)$ be a multigraph. We simply say that G is a *k-graph* if $\operatorname{def}_D(\widetilde{G}) = k$ holds for some nonnegative integer k. In particular, considering the relation between 0-graphs and infinitesimal rigidity given in Proposition 1.1, we say that G is a *body-and-hinge rigid graph* if it is a 0-graph. Recall that $\widetilde{E}$ denotes the edge set of $\widetilde{G}$.

It is not difficult to see the following fact.

Lemma 4.1. *Let G be a body-and-hinge rigid graph. Then, G is 2-edge-connected.*

Remark. Let b and c be positive integers and let $q = b/c$. A multigraph $G = (V, E)$ is called *q-strong* if cG contains b edge-disjoint spanning trees. In this paper, for our particular interest in $q = \frac{D}{D-1}$, we named a $\frac{D}{D-1}$-strong graph as a body-and-hinge rigid graph. Due to the space limitation, please refer to [1, 3–5, 7] for more detailed descriptions of general q-strong graphs.

Minimally body-and-hinge rigid graphs. A *minimal k-graph* is a k-graph in which removing any edge results in a graph that is not a k-graph. In particular, a minimal 0-graph is called a *minimally body-and-hinge rigid graph.* It is not difficult to show that G is not 3-edge-connected. We shall further reveal new combinatorial properties of a minimal k-graph.

Notice that a graph $G = (V, E)$ is a minimal k-graph if and only if $B \cap \widetilde{e} \neq \emptyset$ for any edge $e \in E$ and any base B of $\mathcal{M}(\widetilde{G})$ (introduced in Section 3) by Proposition 3.1. From this observation, it is not difficult to see the following fact concerning the subgraphs of a minimal k-graph.

Lemma 4.2. *Let $G = (V, E)$ be a minimal k-graph for some nonnegative integer k and let $G' = (V', E')$ be a subgraph of G. Suppose G' is a k'-graph for* *some nonnegative integer k'. Then G' is a minimal k'-graph.*

Rigid subgraphs. Let G be a multigraph. We say that a subgraph G' of G is a *rigid subgraph* if G' is a 0-graph, i.e., $\widetilde{G'}$ contains D edge-disjoint spanning trees on the vertex set of G'. In this subsection we claim the following two lemmas for rigid subgraphs.

Lemma 4.3. *Let $G = (V, E)$ be a minimal k-graph for a nonnegative integer k and let $G' = (V', E')$ be a rigid subgraph of G. Then, the graph obtained from G by contracting E' is a minimal k-graph.*

Notice that, for every circuit X of $\mathcal{M}(\widetilde{G})$, $V(X)$ induces a 2-edge-connected subgraph by Lemma 4.1. This fact leads to the following property of a multigraph that is not 2-edge-connected.

Lemma 4.4. *Let $G = (V, E)$ be a minimal k-graph whose edge-connectivity is less than two. Let $\mathcal{P} = \{V_1, V_2\}$ be a partition of V such that $d_G(\mathcal{P}) \leq 1$. Then, $k = k_1 + k_2 + 1$ holds if $d_G(\mathcal{P}) = 1$ and otherwise (i.e. $d_G(\mathcal{P}) = 0$) $k = k_1 + k_2 + D$ holds, where $k_1 = \mathrm{def}_D(\widetilde{G[V_1]})$ and $k_2 = \mathrm{def}_D(\widetilde{G[V_2]})$.*

5 Operations for Minimal k-graphs

In this section we shall discuss simple inductive operations on a minimal k-graph. One operation is the contraction of a *proper* rigid subgraph; $G' = (V', E')$ is called a *proper rigid subgraph* if it is a rigid subgraph of G satisfying $1 < |V'| < |V|$. We have already seen in Lemma 4.3 that the contraction of a rigid subgraph provides a smaller minimal k-graph. Another operation is a so-called splitting off operation. The result will be used to apply an induction in the proof of the Molecular Conjecture. Also as a corollary, we will obtain Theorem 5.4, which must be an interesting result in its own right.

Splitting off operation at a vertex of degree two. We shall examine a splitting off operation that converts a minimal k-graph into the other minimal k-graph of smaller size, which is analogous to that for $2k$-edge-connected graphs [9]. For a vertex v of a graph G, let $N_G(v)$ be a set of vertices adjacent to v in G. A *splitting off at v* is an operation which removes v and then inserts new edges between vertices of $N_G(v)$. We shall consider such an operation only at a vertex v of degree two. Let $N_G(v) = \{a, b\}$. We denote by G^{ab}_v the graph obtained from G by removing v (and the edges incident to v) and then inserting the new edge ab. The operation that produces G^{ab}_v from G is called *the splitting off at v (along ab)*. The following lemma claims that the splitting off does not increase the deficiency but may not preserve the minimality of the resulting graph.

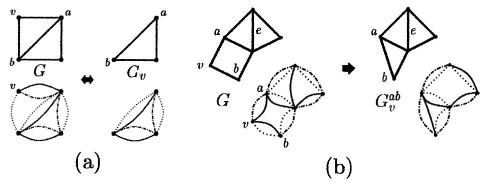

Figure 2: (a)An example of a minimal 0-graph G such that G^{ab}_v is not a minimal 0-graph for $d = 2$ and $D = 3$. Notice that G_v is a 0-graph and hence G^{ab}_v is not minimal. (b) An example of a minimal 0-graph G such that G^{ab}_v is not minimal and also G_v is not a 0-graph for $d = 2$ and $D = 3$. Notice that there exist 3 edge-disjoint spanning trees in $\widetilde{G^{ab}_v}$ that contain no edge of $\widetilde{e}$.

Lemma 5.1. *Let $G = (V, E)$ be a minimal k-graph in which there exists a vertex v of degree 2 with $N_G(v) = \{a, b\}$. Then, G^{ab}_v is either a k-graph or a minimal $(k-1)$-graph.*

Applying Lemma 5.1 to the case of $k = 0$, we see that, for a minimally body-and-hinge rigid graph G, G^{ab}_v is always body-and-hinge rigid. However, as we mentioned, a splitting off may not preserve the minimality of G^{ab}_v. Figure 2 shows such examples, where G_v denotes the graph obtained from G by the removal of v.

Minimal k-graphs having no proper rigid subgraph. As shown in Figure 2 a splitting off does not preserve the minimality of a graph in general. However, if we concentrate on a graph which has no proper rigid subgraph, it can be shown that a splitting off operation has a much clear property. We hence concentrate on graphs having no proper rigid subgraph throughout this subsection.

The following lemma claims the existence of small degree vertices.

Lemma 5.2. *Let $G = (V, E)$ be a 2-edge-connected minimal k-graph which contains no proper rigid subgraph. Then, G has a vertex of degree two. More precisely, if there is a vertex of degree more than two, then G contains a chain $v_1 v_2 \dots v_{d+1}$ of length $d + 1$ (i.e., $v_i v_{i+1} \in E$ for $1 \leq i \leq d$ and $d_G(v_i) = 2$ for $2 \leq i \leq d$).*

Let us start to show the deficiencies of G^{ab}_v, assuming that G contains no proper rigid subgraph.

Lemma 5.3. *Let $G = (V, E)$ be a minimal k-graph which contains no proper rigid subgraph. For any vertex v of degree two with $N_G(v) = \{a, b\}$, the followings hold:*

- *If $k = 0$, then G^{ab}_v is a minimal k-graph.*
- *If $k > 0$, then G^{ab}_v is a minimal $(k-1)$-graph.*

Combining the results obtained so far, it is not difficult to prove the following construction of minimally body-and-hinge rigid graphs.

Theorem 5.4. *Let G be a minimally body-and-hinge rigid graph with $|V| \geq 2$. Then, there exists a sequence $G = G_1, G_2, \ldots, G_m$ of minimally body-and-hinge rigid graphs such that*

- *G_m is a graph consisting of two vertices $\{u, v\}$ and two parallel edges connecting u and v, and*
- *G_{i+1} is obtained from G_i by either the splitting off at a vertex of degree 2 or the contraction of a proper rigid subgraph.*

6 Rigid Panel-and-hinge Realizations

We shall use the following notations to indicate the submatrix of the rigidity matrix $R(G, \mathbf{p})$. Recall the definition of $R(G, \mathbf{p})$ given in Section 2: In $R(G, \mathbf{p})$, consecutive $D-1$ rows are associated with an edge $e \in E$ and consecutive D columns are associated with a vertex $v \in V$. More precisely, the consecutive $D-1$ rows associated with $e = uv \in E$ are described by the $(D-1) \times D|V|$ submatrix: $(\cdots \ \mathbf{0} \ \cdots \ \overset{u}{R(\mathbf{p}(e))} \ \cdots \ \mathbf{0} \ \cdots \ -\overset{v}{R(\mathbf{p}(e))} \ \cdots \ \mathbf{0} \ \cdots)$, where $R(\mathbf{p}(e))$ was defined in Section 2. Let us denote by $R_{G,\mathbf{p}}[e]$ this $(D-1) \times D|V|$-submatrix of $R(G, \mathbf{p})$ given for each $e \in E$. Similarly, let us denote by $R_{G,\mathbf{p}}[v]$ the $(D-1)|E| \times D$-submatrix of $R(G, \mathbf{p})$ induced by the consecutive D columns associated with v. For $F \subseteq E$ and $X \subseteq V$, $R_{G,\mathbf{p}}[F, X]$ denotes the submatrix of $R(G, \mathbf{p})$ induced by the rows of $R_{G,\mathbf{p}}[e]$ for $e \in F$ and the columns of $R_{G,\mathbf{p}}[v]$ for $v \in X$. We need the following technical lemma.

Lemma 6.1. *Let $(G, \mathbf{p})$ be a body-and-hinge framework in $\mathbb{R}^d$. Then, for any vertex $v \in V$, $\operatorname{rank} R_{G,\mathbf{p}}[E, V \setminus \{v\}] = \operatorname{rank} R(G, \mathbf{p})$ holds.*

Generic Nonparallel Realizations. Before providing a proof of the Molecular Conjecture, we need to mention the *generic* property of a panel-and-hinge realization for a simple graph introduced by Jackson and Jordán [8]. For a panel-and-hinge realization $(G, \mathbf{p})$, let $\Pi_{G,\mathbf{p}}(v)$ denote the $(d-1)$-affine subspace (panel) which contains all of the hinges $\mathbf{p}(e)$ of the edges e incident to $v \in V$. For a simple graph G, $(G, \mathbf{p})$ is called a *nonparallel* panel-and-hinge realization if $\Pi_{G,\mathbf{p}}(u)$ and $\Pi_{G,\mathbf{p}}(v)$ are not parallel for any distinct $u, v \in V$. As Jackson and Jordán mentioned in [8, Section 7], each entry of the rigidity matrix $R(G, \mathbf{p})$ of a nonparallel panel-and-hinge realization $(G, \mathbf{p})$ can be described in terms of the coefficients appeared in the equations representing $\Pi_{G,\mathbf{p}}(v)$ for $v \in V$, and hence each minor of the rigidity matrix is a polynomial of these coefficients. If the set of these coefficients is algebraically independent over $\mathbb{Q}$, then the realization is *generic*, i.e., it takes the maximum rank over all nonparallel realizations of G. The rigidity of nonparallel panel-and-hinge realizations thus has a generic property.

It is known that, even though $(G, \mathbf{p})$ has some parallel panels, we can perturb them so that the resulting realization becomes nonparallel without decreasing the rank of the rigidity matrix (see [6, Lemma 4.2] or [8, Lemma 7.1]).

A Proof of the Molecular Conjecture. Let us claim the main theorem of this paper.

Theorem 6.2. *Let $G = (V, E)$ be a minimal k-graph with $|V| \geq 2$ for some nonnegative integer k. Then, there exists a (nonparallel, if G is simple) panel-and-hinge realization $(G, \mathbf{p})$ in $\mathbb{R}^d$ satisfying $\operatorname{rank} R(G, \mathbf{p}) = D(|V| - 1) - k$.*

Before providing a sketch of the proof, let us first write up some corollaries which follow from Theorem 6.2. Since we can convert any k-graph G to a minimal k-graph by greedily removing the redundant edges, the following theorem is easily follows from Theorem 6.2, which proves the Molecular Conjecture in a strong sense combined with Proposition 3.1.

Theorem 6.3. *Let $G = (V, E)$ be a multigraph. Then, G can be realized as a panel-and-hinge framework $(G, \mathbf{p})$ in $\mathbb{R}^d$ satisfying $\operatorname{rank} R(G, \mathbf{p}) = D(|V| - 1) - \operatorname{def}_D(\widetilde{G})$.*

Let us denote the bar-and-joint rigidity matroid in 3-dimensional space by $\mathcal{R}_3(G)$ for a graph G. Jackson and Jordán [5, Conjecture 1.2] have recently showed that, for a graph G of the minimum degree at least two, the Molecular Conjecture is true in 3-dimension if and only if the rank of $\mathcal{R}_3(G^2)$ is equal to $3|V| - 6 - \operatorname{def}_D(5G)$. Combining this result with Theorem 6.3, we found that the above characterization of $\mathcal{R}_3(G^2)$ is true. In particular we obtain the following.

Corollary 6.4. *Let G be a graph of minimum degree at least two. Then, G^2 can be realized as an infinitesimally rigid bar-and-joint framework in 3-dimensional space if and only if $5G$ contains six edge-disjoint spanning trees.*

A Proof of Theorem 6.2. The proof is done by induction on $|V|$. We omit the base case ($|V| = 2$) and let us consider G with $|V| \geq 3$. We shall split the proof into three parts: Lemma 6.5 deals with the case when G is not 2-edge-connected. Lemma 6.6 deals with the case when G is 2-edge-connected and contains a proper rigid subgraph. Lemma 6.7 deals with the rest of the cases. The rest of the description is devoted to the proof of each case. Throughout these lemmas, we will assume the inductive hypothesis on the number of vertices.

The first lemma 6.5 considers the case that G is not 2-edge-connected. This case can be handled rather easily but present a basic strategy of the subsequent arguments.

Lemma 6.5. *Let $G = (V, E)$ be a minimal k-graph which is not 2-edge-connected. Then, there is a (nonparallel, if G is simple) panel-and-hinge realization $(G, \mathbf{p})$ in $\mathbb{R}^d$ satisfying* $\operatorname{rank} R(G, \mathbf{p}) = D(|V|-1)-k$.

Proof. Let us consider the case when G is connected. The case of a disconnected G can be handled in a similar manner. Since G has a cut edge uv, G can be partitioned into two subgraphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ such that $u \in V_1$, $v \in V_2$, $V_1 \cap V_2 = \emptyset$, $V_1 \cup V_2 = V$ and $\delta_G(V_1) = \{uv\}$. Let k_1 and k_2 be the deficiencies of $\widetilde{G_1}$ and $\widetilde{G_2}$, respectively. Then, $k = k_1 + k_2 + 1$ holds by Lemma 4.4 and also G_i is a minimal k_i-graph for each $i = 1, 2$ by Lemma 4.2. By induction hypothesis, we have a (nonparallel, if G_i is simple) panel-and-hinge realization $(G_i, \mathbf{p}_i)$ satisfying $\operatorname{rank} R(G_i, \mathbf{p}_i) = D(|V_i| - 1) - k_i$ for each $i = 1, 2$. Since the choices of $\mathbf{p}_1$ and $\mathbf{p}_2$ are independent of each other and also since the rank of the rigidity matrix is invariant under the rotation of the whole framework, we can take $\mathbf{p}_1$ and $\mathbf{p}_2$ such that $\Pi_{G_1,\mathbf{p}_1}(v_1)$ and $\Pi_{G_2,\mathbf{p}_2}(v_2)$ are not parallel for any pair of $v_1 \in V_1$ and $v_2 \in V_2$. In particular, $\Pi_{G_1,\mathbf{p}_1}(u) \cap \Pi_{G_2,\mathbf{p}_2}(v)$ is a $(d-2)$-affine subspace in $\mathbb{R}^d$. Define the mapping $\mathbf{p}$ as follows: $\mathbf{p}(e) = \mathbf{p}_1(e)$ if $e \in E_1$, $\mathbf{p}(e) = \mathbf{p}_2(e)$ if $e \in E_2$ and otherwise (if $e = uv$) $\mathbf{p}(e) = \Pi_{G_1,\mathbf{p}_1}(u) \cap \Pi_{G_2,\mathbf{p}_2}(v)$. Then, $(G, \mathbf{p})$ is a (nonparallel, if G is simple) panel-and-hinge realization of G. By $\delta_G(V_1) = \{uv\}$, the rigidity matrix $R(G, \mathbf{p})$ can be described as

$$\begin{pmatrix} R_{G_1,\mathbf{p}_1}[E_1, V_1 \setminus \{u\}] & * & * \\ \mathbf{0} & R(\mathbf{p}(uv)) & * \\ \mathbf{0} & \mathbf{0} & R(G_2, \mathbf{p}_2) \end{pmatrix}.$$

Notice that $\operatorname{rank} R_{G_1,\mathbf{p}_1}[E_1, V_1 \setminus \{u\}] = \operatorname{rank} R(G_1, \mathbf{p}) = D(|V_1|-1)-k_1$ holds by Lemma 6.1. Notice also that $\operatorname{rank} R(\mathbf{p}(uv)) = D - 1$ holds since the set of row vectors of $R(\mathbf{p}(uv))$ is a basis of the orthogonal complement of $\langle S(\mathbf{p}(uv))\rangle$ (see Section 2). Hence, by $k = k_1 + k_2 + 1$ and $|V| = |V_1| + |V_2|$, we obtain $\operatorname{rank} R(G, \mathbf{p}) \geq \operatorname{rank} R_{G_1,\mathbf{p}_1}[E_1, V_1 \setminus \{u\}] + \operatorname{rank} R(\mathbf{p}(uv)) + \operatorname{rank} R(G_2, \mathbf{p}_2) = D(|V_1| - 1) - k_1 + (D - 1) + D(|V_2| - 1) - k_2 = D(|V| - 1) - (k_1 + k_2 + 1) = D(|V| - 1) - k$. □

Lemma 6.6. *Let $G = (V, E)$ be a 2-edge-connected minimal k-graph with $|V| \geq 3$. Suppose there exists a proper rigid subgraph in G. Then, there is a (nonparallel, if G is simple) panel-and-hinge realization $(G, \mathbf{p})$ in $\mathbb{R}^d$ satisfying* $\operatorname{rank} R(G, \mathbf{p}) = D(|V|-1)-k$.

Proof. We only describe a sketch of the proof due to the space limitation. Let $G' = (V', E')$ be a proper rigid subgraph in G. Note that G' is a minimal 0-graph by Lemma 4.2 with $1 < |V'| < |V|$. Let $G/E' = ((V \setminus V') \cup \{v^*\}, E/E')$ be the graph obtained from G by contracting the edges of E', where v^* is the new vertex obtained by the contraction. Then, by Lemma 4.3, G/E' is a minimal k-graph with $|(V \setminus V') \cup \{v^*\}| < |V|$. Therefore, by induction hypothesis, there exist panel-and-hinge realizations $(G', \mathbf{p}_1)$ and $(G/E', \mathbf{p}_2)$ satisfying $\operatorname{rank} R(G', \mathbf{p}_1) = D(|V'|-1)$ and $\operatorname{rank} R(G/E', \mathbf{p}_2) = D(|V \setminus V' \cup \{v\}| - 1) - k$. Based on these realizations, we shall construct a realization of G. Intuitively, we shall replace the body associated with v^* in $(G/E', \mathbf{p}_2)$ by $(G', \mathbf{p}_1)$, by regarding $(G', \mathbf{p}_1)$ as a rigid body in $\mathbb{R}^d$. The rank of the resulting framework would become $\operatorname{rank} R(G', \mathbf{p}_1) + \operatorname{rank} R(G/E', \mathbf{p}_2) = D(|V'|-1)+D(|V \setminus V' \cup \{v^*\}|-1)-k = D(|V|-1)-k$. □

The remaining case for proving Theorem 6.2 is the one in which G is 2-edge-connected and has no proper rigid subgraph. In fact, this is actually the most difficult case and our proof becomes quit long. So we shall provide only the storyline.

Lemma 6.7. *Let $G = (V, E)$ be a 2-edge-connected minimal k-graph with $|V| \geq 3$ which contains no proper rigid subgraph. Then, there is a nonparallel panel-and-hinge realization $(G, \mathbf{p})$ in $\mathbb{R}^d$ satisfying* $\operatorname{rank} R(G, \mathbf{p}) = D(|V| - 1)$.

Proof. Let us consider 3-dimensional case for example. Since $d = 3$ and there exists no proper rigid subgraph in G, Lemma 5.2 implies that there exist two vertices of degree two which are adjacent with each other. Let v and a be such two vertices and let $N_G(v) = \{a, b\}$ for some $b \in V$ and $N_G(v) = \{v, c\}$ for some $c \in V$. Lemma 5.3 implies that both G_v^{ab} and G_a^{vc} are minimal k-graphs. Here G_a^{vc} is the graph obtained by performing the splitting-off operation at a along vc. By induction hypothesis, there exist generic nonparallel panel-and-hinge realizations $(G_v^{ab}, \mathbf{q})$ and $(G_a^{vc}, \mathbf{q}_\rho)$ where $\mathbf{q}_\rho$ will be defined later.

We shall construct a realization $(G, \mathbf{p}_1)$ of G based on $(G_v^{ab}, \mathbf{q})$ as follows: Put a new panel for v on the panel $\Pi_{G_v^{ab},\mathbf{q}}(a)$ for a, and then remove the hinge $\mathbf{q}(ab)$ between a and b and join the panel for v and that for b by a new hinge $\mathbf{p}_1(vb)$ instead of $\mathbf{q}(ab)$ (see Figure 3(b)). Finally, join the panel for v and that for a by a hinge as shown in Figure 3(b). Also, another realization $(G, \mathbf{p}_2)$ for G can be constructed symmetrically by changing the role between a and b as shown in Figure 3(c). Although $(G, \mathbf{p}_1)$ and $(G, \mathbf{p}_2)$ are not nonparallel, we will convert them to nonparallel panel-and-hinge realizations by slightly rotating the panel of v without decreasing the rank of the rigidity matrix as we mentioned. In $d = 2$ we can show that at least one of $(G, \mathbf{p}_1)$ and $(G, \mathbf{p}_2)$ attains the desired

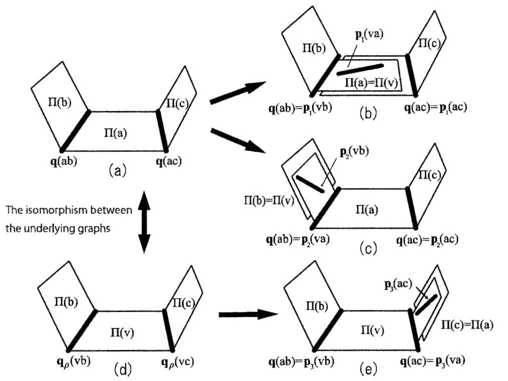

Figure 3: The realizations given in the proof of Lemma 6.7 around v, where the hyperplanes associated with the vertices other than v, a, b, c are omitted. (a)$(G_v^{ab}, \mathbf{q})$, (b)$(G, \mathbf{p}_1)$, (c)$(G, \mathbf{p}_2)$, (d)$(G_a^{vc}, \mathbf{q}_\rho)$ and (e)$(G, \mathbf{p}_3)$.

rank, but this is not always true for $d \geq 3$. Hence, we shall introduce another framework $(G, \mathbf{p}_3)$.

It is not difficult to see that G_a^{vc} is isomorphic to G_v^{ab} and hence there is the realization $(G_a^{vc}, \mathbf{q}_\rho)$ representing the same panel-and-hinge framework as $(G_v^{ab}, \mathbf{q})$, see Figure 3(d). We shall then construct the realization $(G, \mathbf{p}_3)$ based on $(G_a^{vc}, \mathbf{q}_\rho)$ in a similar manner as $(G, \mathbf{p}_1)$, see Figure 3(e). (Again we can convert $(G, \mathbf{p}_3)$ to a nonparallel realization without changing the rank.) Since $(G_a^{vc}, \mathbf{q}_\rho)$ and $(G_v^{ab}, \mathbf{q})$ are the same framework, we expect that the hinge $\mathbf{p}_3(ac)$ would eliminate a nontrivial infinitesimal motion appeared in $(G, \mathbf{p}_1)$ and $(G, \mathbf{p}_2)$. We will show at least one of $(G, \mathbf{p}_1)$, $(G, \mathbf{p}_2)$ and $(G, \mathbf{p}_3)$ attains the desired rank by computing the ranks of the rigidity matrices of these realizations with certain mappings of $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3$. □

Acknowledgment. The first author is supported by the project *New Horizons in Computing*, Grant-in-Aid for Scientific Research on Priority Areas, MEXT Japan, and by Grant-in-Aid for Scientific Research (C), JSPS. The second author is supported by Grant-in-Aid for JSPS Research Fellowships for Young Scientists.

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