# On bicliques and the second clique graph of suspensions

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**Abstract**

The *clique graph* $K(G)$ of a graph $G$ is the intersection graph of the set of all (maximal) cliques of $G$. The *second clique graph* $K^2(G)$ *of* $G$ is defined as $K^2(G) = K(K(G))$. The main motivation for this work is to attempt to characterize the graphs $G$ that maximize $|K^2(G)|$, as has been done for $|K(G)|$ by Moon and Moser in 1965.

The *suspension* $S(G)$ of a graph $G$ is the graph that results from adding two non-adjacent vertices to the graph $G$, that are adjacent to every vertex of $G$. Using a new *biclique* operator $B$ that transforms a graph $G$ into its *biclique graph* $B(G)$, we found the characterization $K^2(S(G)) \cong B(K(G))$. We also found a characterization of the graphs $G$, that maximize $|B(G)|$.

Here, a biclique $(X, Y)$ of $G$ is an ordered pair of subsets of vertices of $G$ (not necessarily disjoint), such that every vertex $x \in X$ is adjacent or equal to every vertex $y \in Y$, and such that $(X, Y)$ is maximal under component-wise inclusion. The biclique graph $B(G)$ of the graph $G$, is the graph whose vertices are the bicliques of $G$ and two vertices $(X, Y)$ and $(X', Y')$ are adjacent, if and only if $X \cap X' \neq \emptyset$ or $Y \cap Y' \neq \emptyset$.

*Keywords:* graph theory, graph dynamics, clique graphs, bicliques.

## 1. Introduction

All our graphs are finite, simple and non-empty. We identify induced subgraphs with their vertex set, in particular, we shall write $x \in G$, instead of $x \in V(G)$. A *clique* of a graph $G$ is a maximal complete subgraph. The *clique graph* $K(G)$ of a graph $G$, is the intersection graph of the set of all cliques of $G$ (i.e. the graph whose vertices are the cliques of $G$ and two vertices are adjacent if and only if they share at least one vertex).

Evidently, the clique operator $K$ can be iterated: $K^{n+1}(G) = K(K^n(G))$, for $n \in \mathbb{N}$. Clique graphs and iterated clique graphs have been studied extensively [12, 17, 21] and have found applications to the study of the Fixed Point Property of partially ordered sets [10] and to Loop Quantum Gravity [18, 19, 20].

If $x$ and $y$ are vertices of the graph $G$ that are adjacent or equal, we shall write $x \simeq y$. We shall denote by $N_G(x)$ and $N_G[x]$ the open neighborhood and closed neighborhood of the vertex $x$, respectively. The subscript will be omitted whenever it is clear from the context which graph is $G$.

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We shall denote by $\overline{G}$ to the complement graph of the graph $G$ and by $K_n$, $I_n$, $C_n$ and $P_n$, to the complete graph, the edgeless graph, the cycle and the path of $n$ vertices, respectively. We also use standard notation for *graph isomorphism* $G \cong H$ and for the *direct product* of graphs $G \times H$. We define the *circle product* by $G \circ H = \overline{\overline{G} \times \overline{H}}$ (in [9] this product is simply denoted as the complementary of the direct product: $\overline{\times}$). Note that in $G \circ H$, the vertices $(g_1, h_1)$ and $(g_2, h_2)$ are adjacent-or-equal if and only if $g_1 \simeq g_2$ in $G$ or $h_1 \simeq h_2$ in $H$; for this reason some authors call this product the *or-product*, hence the symbol used here.

We denote by $G + H$ the *Zykov sum* (also know as the join of graphs) of the graphs $G$ and $H$ (i.e. the graph which is obtained from the disjoint union of $G$ and $H$ by adding all the possible edges between $G$ and $H$). We define the *suspension* $S(G)$ of a graph $G$ by $S(G) = I_2 + G$ and the *d-dimensional octahedral graph* by $O_d = I_2 + I_2 + \cdots + I_2$ ($d$ times).

In this work, we define a *biclique* of a graph $G$ by considering the set $\mathcal{B}_G = \{(X, Y) \in 2^G \times 2^G \mid x \simeq y$, for every $x \in X$ and $y \in Y\}$ and defining a partial order on $\mathcal{B}_G$, by $(X_1, Y_1) \preccurlyeq (X_2, Y_2)$ if and only if $X_1 \subseteq X_2$ and $Y_1 \subseteq Y_2$. A *biclique* $(X, Y)$ of $G$ is a maximal element of $\mathcal{B}_G$ under $\preccurlyeq$. The *biclique graph* $B(G)$ of $G$, is the graph whose vertices are the bicliques of $G$ with $(X_1, Y_1) \simeq (X_2, Y_2)$, if and only if $X_1 \cap X_2 \neq \emptyset$ or $Y_1 \cap Y_2 \neq \emptyset$.

Several variations of a biclique operator have been studied in the literature by Prisner [17], Zelinka [22], Figueroa and Llano [2], and by Groshaus et al. [8, 7, 5, 6, 4]. The variation studied here is new as far as we know.

A well known result from Moon and Moser [13] is that for any given order $n = |G| \geq 2$, the graphs $G$ that maximize the number of cliques (i.e. $|K(G)|$) are defined by $G = H + I_3 + I_3 + \cdots + I_3$, where $H \in \{I_2, I_3, I_2 + I_2, I_4\}$ is taken such that $|H| = |G| - 3\lfloor \frac{n-2}{3} \rfloor$. Intuitively, one would expect that these same graphs also maximize $|K^m(G)|$ for all $m$, but experiments with small graphs show that that is not the case. The experiments (we used GAP and YAGS [3, 1]) show that, for $n \in \{2, 3, \cdots, 9\}$, the number of cliques of $K(G)$ (i.e. $|K^2(G)|$) is maximized when $G = H + I_2 + I_2 + \cdots + I_2$, where $H \in \{I_2, I_3\}$, except for a few expected and understandable exceptions for small $n$ ($I_4$ for $n = 4$ and $I_5$, $C_5$ and $C_4 \cup I_1$ for $n = 5$ also attain the maximum of $|K^2(G)|$ for the given order $n$).

In view of the previous evidence and in an attempt to advance towards a characterization of the graphs maximizing $|K^2(G)|$, we study here the graphs which are suspensions $G = S(G_0) = G_0 + I_2$ and since we characterized $K^2(S(G_0)) \cong B(K(G_0))$ (Theorem 1), we also study the graphs $H$ that maximize $|B(H)|$. Our Theorem 14 gives a full characterization of such graphs.

A preliminary version of this work was published in [16], which only contained proofs for the even order case (next section) and Lemma 4. For the reader's convenience, we include all the proofs here.

## 2. The even order case

Let us characterize first, $K^2(S(G))$ in terms of the biclique operator $B$.

**Theorem 1.** *$K^2(S(G)) \cong B(K(G))$.*

*Proof.* From the definition of $S(G)$, there are vertices $x, y \in S(G) \backslash G$, $x \not\simeq y$, such that $N(x) = N(y) = G$. Note that if $p \in K(S(G))$, then $x \in p$ or $y \in p$, by maximality of $p$, and

$p \setminus \{x\} \in K(G)$ or $p \setminus \{y\} \in K(G)$. Also, if $q \in K(G)$ then $q \cup \{x\}$, $q \cup \{y\} \in K(S(G))$. Define $\tau : B(K(G)) \to K^2(S(G))$ by

$$\tau((X,Y)) = \left(\bigcup_{q\in X}\{q \cup \{x\}\}\right) \cup \left(\bigcup_{q\in Y}\{q \cup \{y\}\}\right).$$

We claim that $\tau$ is an isomorphism of graphs. Let $P = (\bigcup_{i=1}^{r}\{q_i \cup \{x\}\}) \cup (\bigcup_{i=1}^{s}\{q'_i \cup \{y\}\})$ be a clique of $K(S(G))$ with $q_i \in K(G)$ for all $i \in \{1, 2, \ldots, r\}$ and $q'_i \in K(G)$ for all $i \in \{1, 2, \ldots, s\}$, then the ordered pair $W = (\cup_{i=1}^{r}\{q_i\}, \cup_{i=1}^{s}\{q'_i\})$ is a biclique of $K(G)$, it follows that $\tau(W) = P$, thus $\tau$ is surjective.

Let $W_1 = (X_1, Y_1)$ and $W_2 = (X_2, Y_2)$ be bicliques of $K(G)$, if $\tau(W_1) = \tau(W_2)$ then for $A_1 = \bigcup_{q\in X_1}\{q \cup \{x\}\}$ and $A_2 = \bigcup_{q\in X_2}\{q \cup \{x\}\}$ we have that $A_1 = A_2$, hence $X_1 = X_2$. A similar argument shows that $Y_1 = Y_2$, consequently $W_1 = W_2$ and $\tau$ is injective. Finally, the bicliques $W_1$ and $W_2$ are adjacent in $B(K(G))$ if and only if there is a clique $q \in K(G)$ such that $q \in (X_1 \cap X_2) \cup (Y_1 \cap Y_2)$, since the last statement is true if and only if $q \cup \{x\} \in \tau(W_1) \cap \tau(W_2)$ or $q \cup \{y\} \in \tau(W_1) \cap \tau(W_2)$ (i.e. when $\tau(W_1)$ and $\tau(W_2)$ are adjacent in $K^2(S(G))$), we conclude that $\tau$ is an isomorphism. □

It is well known that the clique graph of a Zykov sum is a circle product, $K(G + H) \cong K(G) \circ K(H)$ [14, 15, 11]. The biclique operator also shares this property:

**Theorem 2.** *For any graphs $G$ and $H$, we have: $B(G + H) \cong B(G) \circ B(H)$.*

*Proof.* Define $\phi : B(G+H) \to B(G) \circ B(H)$ by $\phi((G_1 \cup H_1, G_2 \cup H_2)) = ((G_1, G_2), (H_1, H_2))$, where $G_1$ and $G_2$ are subsets of vertices of $G$ and $H_1$ and $H_2$ are subsets of vertices of $H$. We proceed to show that $\phi$ is an isomorphism of graphs.

If $T = ((G_1, G_2), (H_1, H_2)) \in B(G) \circ B(H)$ then $W = (G_1 \cup H_1, G_2 \cup H_2)$ is a biclique of $G + H$, hence $\phi(W) = T$ and $\phi$ is surjective. It is straightforward to verify that $\phi$ is injective. Now, the bicliques $W_1 = (G_1 \cup H_1, G'_1 \cup H'_1)$ and $W_2 = (G_2 \cup H_2, G'_2 \cup H'_2)$ of $G + H$ are adjacent or equal in $B(G + H)$ if and only if $(G_1 \cup H_1) \cap (G_2 \cup H_2) \neq \emptyset$ or $(G'_1 \cup H'_1) \cap (G'_2 \cup H'_2) \neq \emptyset$, but this last statement is true if and only if $(G_1, G'_1) \simeq (G_2, G'_2)$ in $B(G)$ or $(H_1, H'_1) \simeq (H_2, H'_2)$ in $B(H)$, therefore $\phi(W_1) \simeq \phi(W_2)$ in $B(G) \circ B(H)$ (i.e. $\phi$ preserves adjacency). □

Given a graph $G$ and a subset $S \subseteq G$, define $N[S] = \bigcap_{x\in S} N_G[x]$ (with $N[\emptyset] = V(G)$). Note that for every $S \subseteq G$, we have that $(N[N[S]], N[S])$ is a biclique in $B(G)$. Also, for every biclique $(X, Y) \in B(G)$, we have that $(X, Y) = (N[N[X]], N[X])$. Define $\beta : 2^G \to B(G)$ by $\beta(S) = (N[N[S]], N[S])$. Observe that $\beta$ is surjective, and in particular, $|B(G)| \leq 2^{|G|}$. The equality holds exactly when $G$ is an octahedral graph:

**Theorem 3.** *The following statements are equivalent:*

1. *$\beta$ is injective.*
2. *$N[X] \neq N[X']$ for all $X, X' \subseteq G$ with $X \neq X'$.*
3. *$N[G \setminus \{x\}] \neq N[G]$ for all $x \in G$.*
4. *For all $x \in G$, there is some $y \in G$ such that $x \not\simeq y$ and $y \simeq z$ for all $z \in G \setminus \{x\}$.*
5. *$n = |G|$ is even and $G \cong O_d$ for $d = \frac{n}{2}$.*

*Proof.* The implications (1) $\Rightarrow$ (2) $\Rightarrow$ (3) $\Rightarrow$ (4) are straight forward. For (4) $\Rightarrow$ (5), observe that $x$ is the only vertex of $G$ satisfying $y \not\simeq x$ and hence we must have $x \simeq z$ for all $z \in G \setminus \{y\}$. It follows that $G \cong I_2 + I_2 + \cdots + I_2$ ($d$ times). Finally, for (5) $\Rightarrow$ (1), consider two different $X_1, X_2 \subseteq O_d$. Assume, without loss of generality, that $X_1 \setminus X_2 \neq \emptyset$, then there is a vertex $z \in X_1 \setminus X_2$ and a vertex $w \in O_d$ with $w \not\simeq z$. Note that $N[w] = G \setminus \{z\}$, hence $w \in N[X_2]$ and $w \notin N[X_1]$. Therefore $N[X_1] \neq N[X_2]$. $\square$

## 3. The odd order case

By the previous theorem, in the even order case, $|G| = n = 2d$, the maximum value of $|B(G)|$ is $2^n$ and it is achieved exactly when $G \cong O_d$. In the odd order case, $n = 2d + 3$, we shall show that $G$ maximizes $|B(G)|$ if and only if $G \cong I_3 + O_d$ (Theorem 14). Let us start by computing $|B(I_3 + O_d)|$ and hence by obtaining a lower bound for $\max\{|B(G)| : |G| = n\}$.

**Lemma 4.** *Let $n = 2d + 3 = |I_3 + O_d|$, then $|B(I_3 + O_d)| = \frac{5}{8} \cdot 2^n$*

*Proof.* Observe that the bicliques of $I_3$ are: $(\emptyset, I_3)$, $(I_3, \emptyset)$ and $(\{x\}, \{x\})$, for each $x \in I_3$; hence $|B(I_3)| = 5$. By theorems 2 and 3, $B(I_3 + O_d) \cong B(I_3) \circ B(O_d)$, hence $|B(I_3 + O_d)| = |B(I_3) \circ B(O_d)| = |B(I_3)| \cdot |B(O_d)| = 5 \cdot 2^{2d} = \frac{5}{8} \cdot 2^n$. $\square$

In what follows, we shall denote the collections of subsets of $G$ that contain and do not contain the vertex $x \in G$, by $S_x^G$ and $S_{\overline{x}}^G$ respectively. Similarly, the collection of subsets that contain the vertex $x$ and do not contain the vertex $y$ will be denoted by $S_{x,\overline{y}}^G$ and so on. The superscript may be omitted when, from context, it is clear which graph is $G$.

Given a collection $\mathcal{C}$ of subsets of vertices of $G$, we define $\mathbb{B}(\mathcal{C}) = \{\beta(S) \mid S \in \mathcal{C}\}$ (recall that $\beta(S)$ is a biclique of $G$, for every $S \subseteq G$). The following lemma gives a useful upper bound for $|\mathbb{B}(\mathcal{C})|$.

**Lemma 5.** *Let $S$ be a subset of the graph $G$, and let $\mathcal{C}$ be a collection of subsets of $G$ such that for every $X \in \mathcal{C}$, we have that $N[X] \subseteq S$, then $|\mathbb{B}(\mathcal{C})| \leq 2^{|S|}$.*

*Proof.* Recall that for every every $Z \subseteq G$, $(N[N[Z]], N[Z])$ is a biclique of $G$ (and that every biclique has that form). Therefore, a biclique of $G$ is uniquely determined by a subset $N[Z] \subseteq G$. Since for every $X \in \mathcal{C}$, we have that $N[X] \subseteq S$, then $|\mathbb{B}(\mathcal{C})| = |\{N[X] \mid X \in \mathcal{C}\}| \leq 2^{|S|}$. $\square$

From now on, let $\mathcal{G}$ be a graph that maximizes $|B(G)|$ when $|G| = n = 2d + 3$. Note that by Lemma 4, we have that $|B(\mathcal{G})| \geq \frac{5}{8} \cdot 2^n$. We shall use this observation extensively in order to characterize the graph $\mathcal{G}$.

**Lemma 6.** *$\mathcal{G}$ can not have universal vertices (i.e. $N[x] \neq \mathcal{G}$ for all $x \in \mathcal{G}$).*

*Proof.* Suppose that $\mathcal{G}$ has an universal vertex $x$, define $\kappa : S_x \to S_{\overline{x}}$ by $\kappa(S) = S \setminus \{x\}$, note that $\kappa$ is a bijection, moreover, for any $X \in S_x$ we have that $N[X] = N[X \setminus \{x\}] \cap N[x] = N[X \setminus \{x\}] \cap \mathcal{G} = N[X \setminus \{x\}] = N[\kappa(X)]$, this implies that $\mathbb{B}(S_x) = \mathbb{B}(S_{\overline{x}})$, consequently

$$\begin{aligned} |B(\mathcal{G})| &= |\mathbb{B}(2^{\mathcal{G}})| = |\mathbb{B}(S_x \cup S_{\overline{x}})| = |\mathbb{B}(S_x) \cup \mathbb{B}(S_{\overline{x}})| = |\mathbb{B}(S_x)| \\ &\leq |S_x| = 2^{n-1} = \frac{1}{2} \cdot 2^n < \frac{5}{8} \cdot 2^n, \end{aligned}$$

which is a contradiction to the maximality of $\mathcal{G}$ by Lemma 4. Therefore, $\mathcal{G}$ can not have universal vertices. $\square$

Recall that $\overline{\mathcal{G}}$ is the complement of $\mathcal{G}$ (same vertices, complementary set of edges).

**Lemma 7.** *If $\overline{\mathcal{G}}$ has a vertex of degree $r$, then $|B(\mathcal{G})| \leq 2^n\left(\frac{1}{2}+\frac{1}{2^r}\right)$. Hence $\Delta(\overline{\mathcal{G}}) \leq 3$ and if $\Delta(\overline{\mathcal{G}}) = 3$ then $|B(\mathcal{G})| \leq \frac{5}{8}\cdot 2^n$.*

*Proof.* Let $x \in \overline{\mathcal{G}}$ be a vertex of degree $r$. Since for every set $X \in S_x$ we have that $N[X] \subseteq N[x]$, it follows from Lemma 5 that $|\mathbb{B}(S_x)| \leq 2^{|N[x]|} = 2^{n-r}$. Therefore

$$\begin{aligned}|B(\mathcal{G})| &= |\mathbb{B}(S_{\overline{x}}) \cup \mathbb{B}(S_x)| \leq |\mathbb{B}(S_{\overline{x}})| + |\mathbb{B}(S_x)| \leq |S_{\overline{x}}| + |\mathbb{B}(S_x)| \\ &\leq 2^{n-1} + 2^{n-r} = 2^n\left(\frac{1}{2}+\frac{1}{2^r}\right).\end{aligned}$$

For $r \geq 4$, the previous inequality gives $|B(\mathcal{G})| < \frac{5}{8}\cdot 2^n$, which is not possible by Lemma 4 ($\mathcal{G}$ maximizes $|B(G)|$), therefore $\Delta(\overline{\mathcal{G}}) \leq 3$ and if $\Delta(\overline{\mathcal{G}}) = 3$, we must have $|B(\mathcal{G})| \leq \frac{5}{8}\cdot 2^n$. $\square$

**Lemma 8.** *$\overline{\mathcal{G}}$ is the disjoint union of cycles and paths.*

*Proof.* In view of Lemma 6, it will be enough to show that $\Delta(\overline{\mathcal{G}}) \leq 2$. Suppose that $\overline{\mathcal{G}}$ has a vertex $x$ of degree 3 and let $N_{\overline{\mathcal{G}}}(x) = \{y, r, s\}$. We shall show that this assumption leads to $|B(\mathcal{G})| < \frac{5}{8}\cdot 2^n$, a contradiction to Lemma 4 .

Suppose, then, that no vertex of $N_{\overline{\mathcal{G}}}(x)$ has neighbors in $\overline{\mathcal{G}} \setminus \{x, y, r, s\}$, and let $H$ be the induced subgraph of $\mathcal{G}$ with vertices $N_{\overline{\mathcal{G}}}[x]$, then $\mathcal{G} = H + (\mathcal{G} \setminus H)$. Since $|H| = 4$ and $H \neq O_2$, we have that $|B(H)| < |B(O_2)|$ by Theorem 3, it follows from Theorem 2 that

$$\begin{aligned}|B(\mathcal{G})| &= |B(H + (\mathcal{G} \setminus H))| = |B(H) \circ B(\mathcal{G} \setminus H)| = |B(H)||B(\mathcal{G} \setminus H)| \\ &< |B(O_2)||B(\mathcal{G} \setminus H)| = |B(O_2) \circ B(\mathcal{G} \setminus H)| = |B(O_2 + (\mathcal{G} \setminus H))|.\end{aligned}$$

A contradiction to the maximality of $\mathcal{G}$, thus, without loss of generality, there is a vertex $z \in \mathcal{G} \setminus \{x, y, r, s\}$ such that $z$ is not adjacent to $y$. Note that the graph $G_0 = \mathcal{G} \setminus \{x, y\}$ has odd order and by Theorem 3, item 3, there is a vertex $t \in G_0$ such that $U_0 = N_{G_0}[G_0] = N_{G_0}[G_0 \setminus \{t\}]$. Thus, we have the following two cases:

a) Case $t \neq z$. From the proof of Lemma 7, we know that

$$|B(\mathcal{G})| \leq |\mathbb{B}(S_{\overline{x}})| + |\mathbb{B}(S_x)| \leq |S_{\overline{x}}| + |\mathbb{B}(S_x)| \leq 2^{n-1} + 2^{n-3} = \frac{5}{8}\cdot 2^n,$$

with $|\mathbb{B}(S_{\overline{x}})| \leq |S_{\overline{x}}|$. Thus, if we can show that there are two sets $S, S' \in S_{\overline{x}}$ such that $N_{\mathcal{G}}[S] = N_{\mathcal{G}}[S']$, then $\beta(S) = \beta(S')$ and $|\mathbb{B}(S_{\overline{x}})| < |S_{\overline{x}}|$, from this it will follow that $|B(\mathcal{G})| < \frac{5}{8}\cdot 2^n$. For this, let $S = G_0$ and $S' = G_0 \setminus \{t\}$. Since neither $x$ nor $y$ are in $N[S] = N_{\mathcal{G}}[S]$ or in $N[S'] = N_{\mathcal{G}}[S']$, we have that $N[S] = N_{G_0}[S] = U_0$ and $N[S'] = N_{G_0}[S'] = U_0$. Hence $N[S] = N[S']$, which is the desired contradiction.

b) Case $t = z$. Again, from the proof of Lemma 7 we know that

$$|B(\mathcal{G})| \leq |\mathbb{B}(S_{\overline{x}})| + |\mathbb{B}(S_x)| \leq |\mathbb{B}(S_{\overline{x}})| + 2^{|N[x]|} \leq 2^{n-1} + 2^{n-3} = \frac{5}{8} \cdot 2^n,$$

with $|\mathbb{B}(S_x)| \leq 2^{|N[x]|}$. Therefore, if we can show that there are two sets $S,\ S' \in S_x$ such that $N[S], N[S'] \in 2^{N[x]}$ and $N[S] = N[S']$, then $|B(S_x)| < 2^{|N[x]|}$ and it will follow that $|B(\mathcal{G})| < \frac{5}{8} \cdot 2^n$. For this, let $S = G_0 \cup \{x\}$ and $S' = (G_0 \setminus \{t\}) \cup \{x\}$. Again, we have that $N[G_0] = N_{G_0}[G_0]$, thus

$$N[S] = N[G_0] \cap N[x] = N_{G_0}[G_0] \cap N[x] = U_0 \cap N[x] = U_0 \setminus \{r, s\}.$$

Since $r \in S'$, we have that $x \notin N[S']$. Moreover, we have that $N[G_0 \setminus \{t\}] \cap G_0 = N_{G_0}[G_0 \setminus \{t\}] = U_0$, therefore

$$\begin{aligned} N[S'] = N[S'] \setminus \{x\} &= N[G_0 \setminus \{t\}] \cap N(x) = N[G_0 \setminus \{t\}] \cap (G_0 \setminus \{r, s\}) \\ &= (N[G_0 \setminus \{t\}] \cap G_0) \setminus \{r, s\} = U_0 \setminus \{r, s\}. \end{aligned}$$

Hence $N[S] = N[S']$ and $N[S], N[S'] \in 2^{N[x]}$, thus $|B(\mathcal{G})| < \frac{5}{8} \cdot 2^n$, which is the desired contradiction.

It follows that $\Delta(\overline{\mathcal{G}}) \leq 2$. Therefore, $\overline{\mathcal{G}}$ is as claimed. □

From Lemma 8, we have that $\mathcal{G} = \overline{P_{n_1}} + \overline{P_{n_2}} + \cdots + \overline{P_{n_r}} + \overline{C_{m_1}} + \overline{C_{m_2}} + \cdots + \overline{C_{m_s}}$. We leave the calculation of the exact number of bicliques of the complements of paths and cycles as an open problem, nevertheless, an upper bound will suffice to characterize $\mathcal{G}$. For this, we have the following lemmas:

**Lemma 9.** *Let $G$ be a graph with $n = |G|$ and let $\mathcal{C} = \{Z \subseteq G \mid (N[Z], Z) \notin B(G)\}$, then $|B(G)| \leq 2^n - |\mathcal{C}|$.*

*Proof.* Recall that if $(X, Y)$ is a biclique of $G$, then $(X, Y) = (N[N[X]], N[X])$, therefore $(X, Y) = (N[W], W)$ for $W = N[X]$. Since $W \subseteq G$, each set $Z \in \mathcal{C}$ reduces by 1 the total of possible bicliques (which is at most $2^n$), therefore $|B(G)| \leq 2^n - |\mathcal{C}|$. □

The next lemma is useful to construct collections of sets that satisfy Lemma 9.

**Lemma 10.** *Let $G$ be a graph, then for any $Z \subseteq G$ for which there is no set $W \subseteq G$ such that $Z = \cup_{w \in W} N_G(w)$, we have that $(N_{\overline{G}}[\overline{Z}], \overline{Z}) \notin B(\overline{G})$.*

*Proof.* Note that $N_G(x) = \overline{N_{\overline{G}}[x]}$ for any $x \in G$, then, given a set $S \subseteq G$ we have that

$$N_{\overline{G}}[S] = \bigcap_{x \in S} N_{\overline{G}}[x] = \overline{\bigcup_{x \in S} \overline{N_{\overline{G}}[x]}} = \overline{\bigcup_{x \in S} N_G(x)}.$$

Hence, for any $(X, Y) \in B(\overline{G})$, there is a $W \subseteq G$ such that $(X, Y) = (N_{\overline{G}}[N_{\overline{G}}[W]], N_{\overline{G}}[W]) = (N_{\overline{G}}[\overline{Z}], \overline{Z})$, with $Z = \bigcup_{w \in W} N_G(w)$. Hence, for any set $Z$ that doesn't satisfy this condition, we have that $(N_{\overline{G}}[\overline{Z}], \overline{Z}) \notin B(\overline{G})$. □

From Lemma 10 we have that $(N_{\overline{G}}[\overline{Z}], \overline{Z})$ is not a biclique of $\overline{G}$, if $Z$ cannot be expressed as the union of open neighborhoods of $G$. For brevity, we shall call the sets $Z$ that have this property as *non-coverable sets in* $G$. In order to construct non-coverable sets in $G$, we have the following lemma:

**Lemma 11.** *Let $x$ be a vertex of the graph $G$ such that for every $y \in N(x)$, we have that $|N(y) \setminus \{x\}| \geq 1$. Let $Z = \{z_1, \ldots, z_r\}$ be a set of vertices of $G$ such that $Z \supseteq \left(\bigcup_{y \in N(x)} N(y)\right) \setminus \{x\}$. Then every set in the collection $S_{x,\overline{z_1},\ldots,\overline{z_r}}$ is non-coverable in $G$.*

*Proof.* Let $S$ be a set of the collection $S_{x,\overline{z_1},\ldots,\overline{z_r}}$, and let $y$ be a vertex of $G$ such that $N(y) \supseteq \{x\}$. Since $|N(y) \setminus \{x\}| \geq 1$ and $Z$ contains the union of all the open neighborhoods of neighborhoods of $x$ (excluding $x$), there is a vertex $z_i \in Z$ such that $z_i$ is also in $N(y)$, thus, any union of open neighborhoods that includes $x$, also includes some vertex in the set $Z$. Therefore, $S$ is a non-coverable set in $G$. □

Using Lemma 11, we get the following upper bounds for the number of bicliques of complements of paths and cycles:

**Lemma 12.** *The number of bicliques of the complements of paths satisfies:*

1. $|B(\overline{P_2})| = 4 = 2^2$
2. $|B(\overline{P_n})| < \frac{5}{8} \cdot 2^n$ *for* $n \geq 3$.

*Proof.* Let $\{0, \ldots, n-1\}$ be the set of vertices of $P_n$. For $n \leq 4$, is easy to check manually that $|B(\overline{P_2})| = 4$, $|B(\overline{P_3})| = 4 < 5 = \frac{5}{8} \cdot 2^3$ and $|B(\overline{P_4})| = 9 < 10 = \frac{5}{8} \cdot 2^4$.

For $n \geq 5$, the collections $\mathcal{C}_1 = S^{P_n}_{0,\overline{2}}$, $\mathcal{C}_2 = S^{P_n}_{2,\overline{0},\overline{4}}$ and $\mathcal{C}_3 = S^{P_n}_{n-1,\overline{0},\overline{2},\overline{n-3}}$ (if $n = 5$, take $\mathcal{C}_3 = S^{P_n}_{4,\overline{0},\overline{2}}$) are collections of non-coverable sets by Lemma 11, respectively (in particular, $\mathcal{C}_3$ is non-coverable because it is a subset of the collection $S^{P_n}_{n-1,\overline{n-3}}$). Moreover, the collections $\mathcal{C}_1$, $\mathcal{C}_2$ and $\mathcal{C}_3$ are pairwise disjoint because their sets differ in including/excluding the vertices 0 and 2, also note that $|\mathcal{C}_3| > 1$. It follows from Lemmas 9 and 10 that

$$\begin{aligned} |B(\overline{P_n})| &\leq 2^n - |\mathcal{C}_1 \cup \mathcal{C}_2 \cup \mathcal{C}_3| = 2^n - |S^{P_n}_{0,\overline{2}}| - |S^{P_n}_{2,\overline{0},\overline{4}}| - |S^{P_n}_{n-1,\overline{0},\overline{2},\overline{n-3}}| \\ &< 2^n - 2^{n-2} - 2^{n-3} - 1 < \tfrac{5}{8} \cdot 2^n. \end{aligned}$$

□

**Lemma 13.** *The number of bicliques of the complements of cycles satisfies:*

1. $|B(\overline{C_3})| = 5 = \frac{5}{8} \cdot 2^3$.
2. $|B(\overline{C_n})| < \frac{5}{8} \cdot 2^n$ *for* $n \geq 4$.

*Proof.* Let $\{0, \ldots, n-1\}$ be the set of vertices of $C_n$. For $n \leq 5$, is straightforward to check manually that $|B(\overline{C_3})| = 5 = \frac{5}{8} \cdot 2^3$, $|B(\overline{C_4})| = 4 < 10 = \frac{5}{8} \cdot 2^4$ and $|B(\overline{C_5})| = 17 < 20 = \frac{5}{8} \cdot 2^5$.

For $n \geq 6$, the following are collections of non-coverable sets in $C_n$ by Lemma 11:

- $\mathcal{C}_1 = S^{C_n}_{2,\ \overline{0},\ \overline{4}}$.
- $\mathcal{C}_2 = S^{C_n}_{0,\ \overline{(n-2)},\ \overline{2}}$.

- $\mathcal{C}_3 = S^{C_n}_{1,\ \overline{0},\ \overline{2},\ \overline{3},\ \overline{n-1}}$ (non-coverable because of $\overline{n-1}$, 1 and $\overline{3}$).

- $\mathcal{C}_4 = S^{C_n}_{0,\ 1,\ 2,\ \overline{3},\ \overline{n-1}}$ (non-coverable because of $\overline{n-1}$, 1 and $\overline{3}$).

- $\mathcal{C}_5 = S^{C_n}_{3,\ 4,\ \overline{0},\ \overline{2},\ \overline{t}}$. If $n = 6$, take $t = 0$, otherwise take $t = 6$ (non-coverable because of $\overline{2}$, 4 and $\overline{t}$).

- $\mathcal{C}_6 = S^{C_n}_{0,\ 2,\ 3,\ \overline{1},\ \overline{5}}$ (non-coverable because of $\overline{1}$, 3 and $\overline{5}$).

- $\mathcal{C}_7 = S^{C_n}_{2,\ 3,\ 4,\ \overline{0},\ \overline{1},\ \overline{5}}$ (non-coverable because of $\overline{1}$, 3 and $\overline{5}$).

Note that collections $\mathcal{C}_1$, $\mathcal{C}_2$, $\mathcal{C}_3$ and $\mathcal{C}_4$ are pairwise disjoint because their sets differ in including/excluding vertices 0 and 2. The collection $\mathcal{C}_5$ is pairwise disjoint with $\mathcal{C}_1$, $\mathcal{C}_2$ and $\mathcal{C}_4$ because of the vertices 0 and 2, and with $\mathcal{C}_3$ because of the vertex 3. The collection $\mathcal{C}_6$ is pairwise disjoint with $\mathcal{C}_1$, $\mathcal{C}_2$, $\mathcal{C}_3$ and $\mathcal{C}_5$ because of the vertices 0 and 2, and with $\mathcal{C}_4$ because of the vertex 3. The collection $\mathcal{C}_7$ is pairwise disjoint with $\mathcal{C}_2$, $\mathcal{C}_3$, $\mathcal{C}_4$, $\mathcal{C}_5$ and $\mathcal{C}_6$ because of the vertices 0 and 2, and with $\mathcal{C}_1$ because of the vertex 4. Therefore, the collections from $\mathcal{C}_1$ to $\mathcal{C}_7$ are pairwise disjoint.

Note that $|\mathcal{C}_7| \geq 1$, it follows from Lemmas 9 and 10 that

$$\begin{aligned}
|B(\overline{C_n})| \ &\leq 2^n - |\cup_{i=1}^{7} \mathcal{C}_i| = 2^n - \left(\textstyle\sum_{i=1}^{7} |\mathcal{C}_i|\right) \leq 2^n - (|S^{C_n}_{2,\ \overline{0},\ \overline{4}}| \\
&+|S^{C_n}_{0,\ \overline{(n-2)},\ \overline{2}}| + |S^{C_n}_{1,\ \overline{0},\ \overline{2},\ \overline{3},\ \overline{n-1}}| + |S^{C_n}_{0,\ 1,\ 2,\ \overline{3},\ \overline{n-1}}| \\
&+|S^{C_n}_{3,\ 4,\ \overline{0},\ \overline{2},\ \overline{t}}| + |S^{C_n}_{0,\ 2,\ 3,\ \overline{1},\ \overline{5}}| + |S^{C_n}_{2,\ 3,\ 4,\ \overline{0},\ \overline{1},\ \overline{5}}|) \\
&\leq 2^n - (2 \cdot 2^{n-3} + 4 \cdot 2^{n-5} + 1) < \tfrac{5}{8} \cdot 2^n.
\end{aligned}$$

□

**Theorem 14.** *Let $\mathcal{G}$ be a graph of order $n > 1$, maximizing $|B(\mathcal{G})|$. Then, if $n = 2d$, we have that $\mathcal{G} \cong O_d$; otherwise, $n = 2d + 3$ and $\mathcal{G} \cong I_3 + O_d$.*

*Proof.* The even order case, $n = 2d$, is covered by Theorem 3. For the odd order case, $n = 2d + 3$, we have that $\mathcal{G} = \overline{C_{m_1}} + \overline{C_{m_2}} + \cdots + \overline{C_{m_s}} + \overline{P_{n_1}} + \overline{P_{n_2}} + \cdots + \overline{P_{n_r}}$ by Lemma 8 and from Theorem 2, we have that

$$\begin{aligned}
|B(\mathcal{G})| &= |B(\overline{C_{m_1}} + \overline{C_{m_2}} + \cdots + \overline{C_{m_s}} + \overline{P_{n_1}} + \overline{P_{n_2}} + \cdots + \overline{P_{n_r}})| \\
&= |B(\overline{C_{m_1}}) \circ B(\overline{C_{m_2}}) \circ \cdots \circ B(\overline{C_{m_s}}) \circ B(\overline{P_{n_1}}) \circ B(\overline{P_{n_2}}) \circ \cdots \circ B(\overline{P_{n_r}})| \\
&= |B(\overline{C_{m_1}})| \cdot |B(\overline{C_{m_2}})| \cdots |B(\overline{C_{m_s}})| \cdot |B(\overline{P_{n_1}})| \cdot |B(\overline{P_{n_2}})| \cdots |B(\overline{P_{n_r}})|.
\end{aligned}$$

Since $I_2 = \overline{P_2}$, $I_3 = \overline{C_3}$ and $O_d = I_2 + I_2 + \cdots + I_2$ ($d$ times), it follows from lemmas 12 and 13 that $\mathcal{G}$ can only attain the maximum when $\mathcal{G} \cong I_3 + I_2 + I_2 + \cdots + I_2 = I_3 + O_d$ as claimed. □

Neumann-Lara proved in [14] that the clique graph of the $d$-dimensional octahedral graph $O_d$, is again an octahedral graph (indeed: $K(O_d) \cong O_{2^{d-1}}$). Since $K^2(S(G)) \cong B(K(G))$ by Theorem 1, it follows that $K^2(O_d) = K^2(S(O_{d-1})) \cong B(K(O_{d-1})) \cong B(O_{2^{d-2}})$. This result, together with Theorem 14, suggest that if $G$ has even order, the graphs maximizing $|K^2(G)|$

are the same as those maximizing $|B(G)|$ (except when $n = 4$, in this case, $I_4$ also maximizes $|K^2(G)|$). Certainly, we have the following bound:

$$|K^2(G)| \geq |K^2(O_d)| = |B(O_{2^{d-2}})| = 2^{2^{d-1}} = \sqrt{2}^{\sqrt{2}^n}.$$

For the odd order case, the experimental evidence mentioned before, suggest that the graphs maximizing $|K^2(G)|$ are also the same as those maximizing $|B(G)|$ (except for the few exceptions mentioned earlier in Section 1).

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