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HARARY INDEX OF THE k-TH POWER OF A GRAPH

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The k-th power of a graph G, denoted by G^k, is a graph with the same set of vertices as G, such that two vertices are adjacent in G^k if and only if their distance in G is at most k. The Harary index $\mathbf{H}$ is the sum of the reciprocal distances of all pairs of vertices of the underlying graph. Lower and upper bounds on $\mathbf{H}(G^k)$ are obtained. A Nordhaus–Gaddum type inequality for $\mathbf{H}(G^k)$ is also established.

1. INTRODUCTION

In this paper, we consider finite undirected simple connected graphs. Let G be such a graph with vertex set $V = V(G)$ and edge set $E = E(G)$. Then the order and size of G are $n = |V|$ and $m = |E|$, respectively. The *degree* $\deg(u) = \deg_G(u)$ of a vertex $u \in V$ is the number of edges incident to u in G. The *maximum degree* in the graph G will be denoted by $\triangle = \triangle(G)$. The *distance* $\mathrm{dist}(u, v) = \mathrm{dist}_G(u, v)$ between two vertices u and v of G is the length of a shortest path connecting them in it. The maximum value of these numbers is said to be the *diameter* of G, denoted by $\mathrm{diam}(G)$.

The *k-th power* G^k of a graph G is a graph with vertex set V, such that two vertices are adjacent in G^k if and only if their distance in G is at most k. In particular, $G^k = G$ if $k = 1$. The *complement* $\overline{G}$ of G is a simple graph with vertex set V, in which two distinct vertices are adjacent if and only if they are not adjacent in G. The *join* $G_1 + G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all edges joining V_1 and V_2. Let K_n, P_n and S_n be respectively the complete graph, the path and

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the star of order n. Other terminology and notations needed will be introduced as it naturally occurs in the following and we use [**3**] for those not defined here.

The Harary index $\mathbf{H}(G)$ has been introduced in 1993 independently by Plavšić et al. [**9**] and Ivanciuc et al. [**6**]. For a connected graph G with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ it is defined as

$$\mathbf{H}(G) = \sum_{1 \le i < j \le n} \frac{1}{\mathrm{dist}_G(v_i, v_j)}.$$

This index was named in honor of Professor Frank Harary on the occasion of his 70th birthday. Details on the applications of the Harary index can be found in the survey [**7**], whereas we can find details on its mathematical properties in [**5, 10**] and the references cited therein.

Let I be an invariant of G. We denote by $\overline{I}$ the same invariant pertaining to $\overline{G}$. The following relations

$$L_1(n) \le I + \overline{I} \le U_1(n) \qquad \text{and} \qquad L_2(n) \le I \cdot \overline{I} \le U_2(n)$$

are referred to as *Nordhaus–Gaddum type inequalities* for the graph invariant I. Here $L_1(n)$ and $L_2(n)$ are the lower bounding functions of the order n, and $U_1(n)$ and $U_2(n)$ the upper bounding functions of the order n. It were Nordhaus and Gaddum [**8**] who first discovered such results for the chromatic number. They proved:

Theorem 1.1. *Let G be a connected graph of order n. Then*

$$2\sqrt{n} \le \chi + \overline{\chi} \le n + 1 \qquad \textit{and} \qquad n \le \chi \cdot \overline{\chi} \le \left\lfloor \left(\frac{n+1}{2} \right)^2 \right\rfloor$$

where χ denotes the chromatic number of G.

Since then many results of this kind were obtained; for a survey see [**2**]. We list here a few, relevant for the present paper.

The Wiener and hyper-Wiener indices of a connected graph G are defined as

$$\mathbf{W}(G) = \sum_{1 \le i < j \le n} \mathrm{dist}_G(v_i, v_j)$$

$$\mathbf{WW}(G) = \sum_{1 \le i < j \le n} \frac{1}{2} \left[\mathrm{dist}_G(v_i, v_j) + \mathrm{dist}_G(v_i, v_j)^2 \right]$$

respectively.

Theorem 1.2. (An and Wu [**1**]) *Let G be a connected graph of order $n \ge 5$, having a connected complement $\overline{G}$. Then*

$$2\binom{n}{2} \le \mathbf{W}(G^k) + \mathbf{W}(\overline{G}^k) \le \mathbf{W}(P_n^k) + \mathbf{W}(\overline{P}_n^k) = \binom{n}{2} + \sum_{i=1}^{n-1} \left\lceil \frac{i}{k} \right\rceil (n - i).$$

Theorem 1.3. (Zhang et al. [**12**]) *Let G be a connected graph of order $n \geq 5$, having a connected complement $\overline{G}$. Then*

$$2\left(1+\left\lfloor\frac{1}{k}\right\rfloor\right)\binom{n}{2} \leq \mathbf{WW}(G^k)+\mathbf{WW}\big(\overline{G}^k\big) \leq \mathbf{WW}(P_n^k)+\mathbf{WW}\big(\overline{P}_n^k\big).$$

Theorem 1.4. (Zhou et al. [**13**]) *Let G be a connected graph of order $n \geq 5$, having a connected complement $\overline{G}$. If* $\operatorname{diam}(\overline{G}) = 2$, *then*

$$1+\frac{(n-1)^2}{2}+n\sum_{i=1}^{n-1}\frac{1}{i} = \mathbf{H}(P_n)+\mathbf{H}\big(\overline{P}_n\big) \leq \mathbf{H}(G)+\mathbf{H}(\overline{G}) \leq \frac{3n(n-1)}{4}.$$

The lower and upper bounds are sharp.

Motivated by the above theorems, in this paper we obtain similar results for the Harary index of the k-th power of a graph.

2. SOME BOUNDS FOR HARARY INDEX

2.1. Bounds for the Harary index of G^k

Let T be a tree of order n, we start from the fact due to [**4**]

$$\mathbf{H}(P_n) \leq \mathbf{H}(T) \leq \mathbf{H}(S_n) \tag{1}$$

with left equality if and only if $T \cong P_n$, and right equality if and only if $T \cong S_n$. Here we present an analogous result for the Harary index of power graphs.

We need the following Lemma:

Lemma 2.1. (An and Wu [**1**]) *Let u, v be two vertices of a connected graph G. Then* $\operatorname{dist}_{G^k}(u,v) = \lceil \operatorname{dist}_G(u,v)/k \rceil$.

Theorem 2.2. *For any tree T of order n,* $\mathbf{H}(P_n^k) \leq \mathbf{H}(T^k) \leq \mathbf{H}(S_n^k)$.

Proof. Note that $\operatorname{diam}(S_n) = 2$, so $\operatorname{diam}(S_n^k) = 1$ and then $\mathbf{H}(S_n^k) = \binom{n}{2}$. The upper bound holds and it is best possible.

Let $P_n = vv_1v_2\dots v_{n-1}$ be a path of order n. We prove that $\mathbf{H}(P_n^k) \leq \mathbf{H}(T^k)$ by induction on n. It is obvious that the claim holds for $n \leq 4$. Let T be a tree of order $n \geq 5$ and let $P_{d+1} = uu_1u_2\dots u_d$ be a longest path in it. Then $\deg_T(u) = 1$ and $T-u$ is a tree of order $n-1$. Set $V(T) = \{u, u_1, \dots, u_d\} \cup \{u_{d+1}, u_{d+2}, \dots, u_{n-1}\}$. Then $\operatorname{dist}_T(u, u_j) \leq d \leq n-1$ for $j = d+1, d+2, \dots, n-1$. Hence $\operatorname{dist}_T(u, u_i) \leq \operatorname{dist}_{P_n}(v, v_i)$ for $i = 1, 2, \dots, n-1$. By Lemma 2.1, we have $\operatorname{dist}_{T^k}(u, u_i) \leq \operatorname{dist}_{P_n^k}(v, v_i)$ for $i = 1, 2, \dots, n-1$. Thus, by the induction hypothesis, we get

$$\begin{aligned}\mathbf{H}(T^k) &= \sum_{i=1}^{n-1} \mathrm{dist}_{T^k}(u, u_i) + \mathbf{H}((T-u)^k)\\ &\geq \sum_{i=1}^{n-1} \mathrm{dist}_{P_n^k}(u, u_i) + \mathbf{H}((P_n - v)^k) = \mathbf{H}(P_n^k).\end{aligned}$$

This completes the proof.

Corollary 2.3. *Let G be a connected graph of order n. Then $\mathbf{H}(P_n^k) \leq \mathbf{H}(G^k)$.*

Proof. Let T be a spanning tree of G. It is obvious that $\mathrm{dist}_G(u,v) \leq \mathrm{dist}_T(u,v)$ for any two vertices u and v of G. By Lemma 2.1, $\mathrm{dist}_{G^k}(u,v) \leq \mathrm{dist}_{T^k}(u,v)$, and therefore $\mathbf{H}(T^k) \leq \mathbf{H}(G^k)$. By Theorem 2.2, $\mathbf{H}(P_n^k) \leq \mathbf{H}(G^k)$ as desired.

2.2. Bounds for the Harary index of G

Let $(G_1 \cdot G_2)(a_1 \cdot a_2)$ denote the *splice* of two connected graphs G_1 and G_2, obtained by identifying the vertices $a_1 \in V_1$ and $a_2 \in V_2$. Let n and d be two integers such that $n > d$. Let $T_{n,d} = (K_{1,d} \cdot P_{n-d})(b_1 \cdot b_2)$ be the graph obtained by identifying a leaf b_1 of the star $K_{1,d}$ with a leaf b_2 of the path P_{n-d}. It is immediately seen that the $T_{n,d}$ has maximum degree d and order n. In particular, if $d = 2$, then $T_{n,d} \cong P_n$. By direct computation, the Harary index of $T_{n,d}$ can be written as

$$\mathbf{H}(T_{n,d}) = d + \frac{1}{2}\binom{d-1}{2} + \frac{d-1}{n-d+1} + n\sum_{i=2}^{n-d}\frac{1}{i}.$$

For the sake of simplicity, in what follows we denote $\mathbf{H}(T_{n,d})$ by $\Phi(n,d)$.

Lemma 2.4. *For $2 \leq d \leq n-1$, $\Phi(n,d)$ is an increasing function of d.*

Proof. We consider the difference $\Phi(n,d) - \Phi(n,d+1)$ and verify that it is negative–valued:

$$\begin{aligned}\Phi(n,d) - \Phi(n,d+1) &= -1 + \frac{1}{2}\left[\binom{d-1}{2} - \binom{d}{2}\right]\\ &\quad + \left[\frac{d-1}{n-d+1} - \frac{d}{n-d}\right] + n\left[\sum_{i=2}^{n-d}\frac{1}{i} - \sum_{i=2}^{n-d-1}\frac{1}{i}\right]\\ &= -1 + \frac{1}{2}\left[\binom{d-1}{2} - \binom{d}{2}\right] + \left[\frac{d-1}{n-d+1} - \frac{d}{n-d}\right] + \frac{n}{n-d}\\ &= \frac{d-1}{n-d+1} - \frac{d-1}{2} < \frac{d-1}{2} - \frac{d-1}{2} = 0.\end{aligned}$$

The second inequality above holds because $2 \leq d \leq n-1$, that is $1/(n-d+1) < 1/2$. This completes the proof.

Lemma 2.5. *For $i = 1, 2$, let T_i be a tree of order n_i, and let x_i be its specified vertex. Then $\mathbf{H}((T_1 \cdot T_2)(x_1 \cdot x_2))$ is minimized if $T_i \cong P_{n_i}$ and x_i is a leaf of T_i.*

Proof. The Harary index of $(T_1 \cdot T_2)(x_1 \cdot x_2)$ satisfies

$$\mathbf{H}((T_1 \cdot T_2)(x_1 \cdot x_2)) = \mathbf{H}(T_1) + \mathbf{H}(T_2) + \sum_{x \in V(T_1), y \in V(T_2)} \frac{1}{\mathrm{dist}(x, y)}.$$

We complete the proof by recalling the relations (1). □

We now give two auxiliary transformations that decrease the Harary index.

Transformation I. Let T be a tree and v one of its vertex with maximum degree. Let T_0 be a component of $T - v$. By replacing T_0 with a path of the same order and the same pendent vertex as T_0 under the definition of splice, we obtain a new tree $T^{'}$. By Lemma 2.5, the transformation $T \to T^{'}$ decreases the Harary index.

Transformation II. Consider the trees T_1 and T_2 depicted in Fig. 1. Note that:

$$T_1[\{v\} \cup V(P_a) \cup V(P_b)] = P_{a+b+1} = T_2[\{v\} \cup V(P_a) \cup V(P_b)].$$

We get $\mathrm{dist}_{T_1}(x, y) = \mathrm{dist}_{T_2}(x, y)$ if $x \in \{v\} \cup V(P_a)$ and $y \notin \{v\} \cup V(P_a) \cup V(P_b)$; and $\mathrm{dist}_{T_1}(x, y) \leq \mathrm{dist}_{T_2}(x, y)$ if $x \in V(P_b)$ and $y \notin \{v\} \cup V(P_a) \cup V(P_b)$. This implies that the transformation $T_1 \to T_2$ decreases the Harary index.

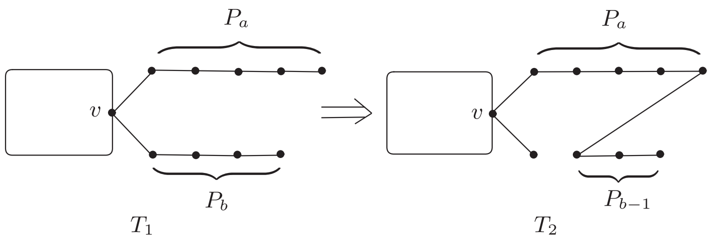

Figure 1. A transformation that decreases the value of the Harary index.

Theorem 2.6. *Let G be a connected graph of order n and $\Delta(G) \geq d \geq 2$. Then $\mathbf{H}(G) \geq \Phi(n, d)$, with equality if and only if $G \cong T_{n,d}$.*

Proof. By Lemma 2.4, we get $\Phi(n, d+1) \geq \Phi(n, d)$. Without loss of generality, we may assume that $\Delta(G) = d$. Then it suffices to prove that $\mathbf{H}(G) \geq \Phi(n, d)$ and that the equality holds if and only if $G \cong T_{n,d}$.

Let T be a spanning tree of G with $\Delta(T) = \Delta(G) = d$, then $\mathbf{H}(T) \leq \mathbf{H}(G)$. Let v be a vertex of T with maximum degree, and $x_{11}, x_{21}, \ldots, x_{d1}$ be its neighbors in T. Let for each $i = 1, 2, \ldots, d$, T_i be the component of $T - v$ containing x_{i1}. Let T_i be of order n_i. By replacing each component T_i by a path $P_{n_i} = x_{i1} x_{i2} \ldots x_{in_i}$ with the same pendent vertex x_{i1}, we obtain a new tree T^{*}. By Transformation I, we know that $\mathbf{H}(T^{*}) \leq \mathbf{H}(T)$.

Without loss of generality, assume that $T^* \neq T_{n,d}$, since otherwise we are done. For the sake of simplicity, assume that $n_1 \geq n_2 \geq \cdots \geq n_d$.. Let $T^{**} = T^* - x_{21}x_{22} + x_{22}x_{1n_1}$. It is easy to show that $\Delta(T^{**}) = d$ and by Transformation II, $\mathbf{H}(T^{**}) \leq \mathbf{H}(T^*)$. If the resulting new tree $T^{**} \ncong T_{n,d}$, repeating Transformation II, we must arrive at the tree $T_{n,d}$.

3. NORDHAUS–GADDUM TYPE INEQUALITY FOR HARARY INDEX

Let $S_{p,q}$ denote the *double star*, obtained from S_p and S_q by connecting the center of S_p with that of S_q. The following fact can be found in [**11**].

Lemma 3.1. (Zhang and Wu [**11**]) *Let G be a connected graph with a connected complement. Then*
(1) *if* $\mathrm{diam}(G) > 3$, *then* $\mathrm{diam}(\overline{G}) = 2$.
(2) *if* $\mathrm{diam}(G) = 3$, *then $\overline{G}$ has a spanning subgraph which is a double star.*

Note that for $n = 4$ there exists only one connected graph P_4 with connected complement $\overline{P}_4 \cong P_4$. It is obvious that if $k = 1$, then $\mathbf{H}(P_4) + \mathbf{H}\big(\overline{P}_4\big) = 26/3$. If $k = 2$, then $\mathbf{H}(P_4^2) + \mathbf{H}\big(\overline{P}_4^2\big) = 11$. If $k \geq 3$, then $\mathbf{H}(P_4^k) + \mathbf{H}\big(\overline{P}_4^k\big) = 12$ since $P_4^k \cong K_4 \cong \overline{P}_4^k$.

In the following we calculate the value of $\mathbf{H}(P_n^k) + \mathbf{H}\big(\overline{P}_n^k\big)$ for $n \geq 5$. Let $P_n = v_1v_2\dots v_n$. Then for any j , $1 \leq j \leq n-1$, we have $\mathrm{dist}_{P_n^k}(v_i, v_{i+j}) = \lceil j/k \rceil$. Hence,

$$\mathbf{H}(P_n^k) = \sum_{j=1}^{n-1}\sum_{i=1}^{n-j} \frac{1}{\mathrm{dist}_{P_n^k}(v_i, v_{i+j})} = \sum_{j=1}^{n-1}\sum_{i=1}^{n-j} \frac{1}{\left\lceil \frac{j}{k} \right\rceil} = \sum_{j=1}^{n-1} \frac{1}{\left\lceil \frac{j}{k} \right\rceil}(n-j).$$

On the other hand, $\mathbf{H}(\overline{P}_n^k) = \binom{n}{2}$ since $\mathrm{diam}(\overline{P}_n^k) = 1$ for $k \geq 3$. Thus,

$$\mathbf{H}(P_n^k) + \mathbf{H}(\overline{P}_n^k) = \binom{n}{2} + \sum_{j=1}^{n-1} \frac{1}{\left\lceil \frac{j}{k} \right\rceil}(n-j). \tag{2}$$

From the above results and Corollary 2.3, we obtain the following result:

Corollary 3.2. *Let G be a connected graph of order $n \geq 5$. If* $\mathrm{diam}(\overline{G}) = 2$, *then* $\mathbf{H}(P_n^k) + \mathbf{H}\big(\overline{P}_n^k\big) \leq \mathbf{H}(G^k) + \mathbf{H}\big(\overline{G}^k\big)$.

Let $\mathbb{E}$ denote the set of even numbers in $[n-1] = \{1, 2, \dots, n-1\}$ and $\mathbb{O}$ that of odd numbers in $[n-1]$.

Lemma 3.3. *Let G be a connected graph of order $n \geq 9$ having a connected complement $\overline{G}$. Then* $\mathbf{H}(P_n^2) + \mathbf{H}\big(\overline{P}_n^2\big) \leq \mathbf{H}(G^2) + \mathbf{H}\big(\overline{G}^2\big)$.

Proof. Let $\Phi(G) = \mathbf{H}(G^2) + \mathbf{H}(\overline{G}^2) - [\mathbf{H}(P_n^2) + \mathbf{H}(\overline{P}_n^2)]$. It is sufficient to show that $\Phi(G) \geq 0$. By Lemma 3.1 and Corollary 3.2 we need to consider only the case $\mathrm{diam}(G) = \mathrm{diam}(\overline{G}) = 3$. In this case, $\mathrm{diam}(G^2) = \mathrm{diam}(\overline{G}^2) = 2$. Let t_i and $\overline{t}_i$ be, respectively, the number of vertex pairs at distance i in G and $\overline{G}$. Note that $t_1 + \overline{t}_1 = \binom{n}{2}$, $t_2 + t_3 = \overline{t}_1$ and $\overline{t}_2 + \overline{t}_3 = t_1$. Then

$$\mathbf{H}(G^2) + \mathbf{H}(\overline{G}^2) = \left(t_1 + t_2 + \frac{1}{2}t_3\right) + \left(\overline{t}_1 + \overline{t}_2 + \frac{1}{2}\overline{t}_3\right) = \frac{3}{2}\binom{n}{2} + \frac{1}{2}(t_2 + \overline{t}_2).$$

By Lemma 3.1, there exists a spanning subgraph, say $S_{p,n-p}$, in G and a spanning subgraph, say $S_{q,n-q}$, in $\overline{G}$, respectively. It is easily seen that

$$t_3 + \overline{t}_3 \leq (p-1)(n-p-1) + (q-1)(n-q-1) \leq \frac{(n-2)^2}{2}.$$

Hence $t_2 + \overline{t}_2 = \binom{n}{2} - (t_3 + \overline{t}_3) \geq (3n-4)/2$.

We consider the following two cases depending on parity of order n.

Case 1. n is odd.

By Eq. (2) we have

$$\begin{aligned}
\mathbf{H}(\overline{P}_n^2) + \mathbf{H}(P_n^2) &= \binom{n}{2} + \sum_{i=1}^{n-1} \frac{n-i}{\left\lceil \frac{i}{2} \right\rceil} = \binom{n}{2} + 2\sum_{i \in \mathbb{E}} \frac{n-i}{i} + 2\sum_{i \in \mathbb{O}} \frac{n-i}{i+1} \\
&= \binom{n}{2} + 2n\sum_{i \in \mathbb{E}} \frac{1}{i} - 2\sum_{i \in \mathbb{E}} 1 + 2n\sum_{i \in \mathbb{O}} \frac{1}{i+1} - 2\sum_{i \in \mathbb{O}} \frac{i}{i+1} \\
&= \binom{n}{2} + 4n\sum_{i \in \mathbb{E}} \frac{1}{i} - 2\sum_{i \in \mathbb{E}} 1 - 2\sum_{i \in \mathbb{O}} \frac{i}{i+1} \\
&= \binom{n}{2} - 2(n-1) + (4n+2)\sum_{i \in \mathbb{E}} \frac{1}{i}.
\end{aligned}$$

Hence

$$\begin{aligned}
\Phi(G) &= \frac{3}{2}\binom{n}{2} + \frac{1}{2}(t_2 + \overline{t}_2) - \left[\binom{n}{2} - 2(n-1) + (4n+2)\sum_{i \in \mathbb{E}} \frac{1}{i}\right] \\
&\geq \frac{3}{2}\binom{n}{2} + \frac{3n-4}{4} - \left[\binom{n}{2} - 2(n-1) + (4n+2)\sum_{i \in \mathbb{E}} \frac{1}{i}\right] \\
&= \frac{n^2 + 10n - 12}{4} - (4n+2)\sum_{i \in \mathbb{E}} \frac{1}{i}.
\end{aligned}$$

If $n = 9$, then

$$\Phi(G) \geq \frac{9^2 + 10 \times 9 - 12}{4} - (4 \times 9 + 2)\left(\frac{1}{2} + \frac{1}{4} + \frac{1}{6} + \frac{1}{8}\right) = \frac{1}{6} > 0.$$

If $n \geq 10$, then

$$\sum_{i \in \mathbb{E}} \frac{1}{i} \leq \frac{n}{24} + \frac{77}{120},$$

since

$$\begin{aligned}\sum_{i \in \mathbb{E}} \frac{1}{i} &\leq \left(\frac{1}{2} + \frac{1}{4} + \frac{1}{6} + \frac{1}{8} + \frac{1}{10}\right) + \sum_{i \in \mathbb{E}^-} \frac{1}{i} \\ &\leq \frac{137}{120} + \sum_{i \in \mathbb{E}^-} \frac{1}{12} = \frac{137}{120} + \frac{1}{12} \times \frac{n-12}{2} = \frac{n}{24} + \frac{77}{120},\end{aligned}$$

where $\mathbb{E}^- = \mathbb{E} \setminus \{2, 4, 6, 8, 10\}$. Hence

$$\Phi(G) = \frac{n^2 + 10n - 12}{4} - (4n+2)\left(\frac{n}{24} + \frac{77}{120}\right) = \frac{5n^2 - 9n + 257}{60} > 0.$$

Case 2. n is even.

By Eq. (2) we have

$$\begin{aligned}\mathbf{H}(\overline{P}_n^2) + \mathbf{H}(P_n^2) &= \binom{n}{2} + \sum_{i=1}^{n-1} \frac{n-i}{\left\lceil \frac{i}{2} \right\rceil} = \binom{n}{2} + 2\sum_{i \in \mathbb{E}} \frac{n-i}{i} + 2\sum_{i \in \mathbb{O}} \frac{n-i}{i+1} \\ &= \binom{n}{2} + 2n\sum_{i \in \mathbb{E}} \frac{1}{i} - 2\sum_{i \in \mathbb{E}} 1 + 2n\sum_{i \in \mathbb{O}} \frac{1}{i+1} - 2\sum_{i \in \mathbb{O}} \frac{i}{i+1} \\ &= \binom{n}{2} + 2n\sum_{i \in \mathbb{E}} \frac{1}{i} - 2\sum_{i \in \mathbb{E}} 1 + \left[2n \sum_{i \in \mathbb{O}^-} \frac{1}{i+1} + \frac{2n}{(n-1)+1}\right] \\ &\quad - \left[2\sum_{i \in \mathbb{O}} 1 + 2\sum_{i \in \mathbb{O}^-} \frac{1}{i+1} + \frac{2}{(n-1)+1}\right] \\ &= \binom{n}{2} + \frac{2}{n} + 2 - 2(n-1) + (4n+2)\sum_{i \in \mathbb{E}} \frac{1}{i}\ ,\end{aligned}$$

where $\mathbb{O}^- = \mathbb{O} \setminus \{n-1\}$. Hence

$$\begin{aligned}\Phi(G) &= \frac{3}{2}\binom{n}{2} + \frac{1}{2}(t_2 + \overline{t}_2) - \left[\binom{n}{2} + \frac{2}{n} + 2 - 2(n-1) + (4n+2)\sum_{i \in \mathbb{E}} \frac{1}{i}\right] \\ &\geq \frac{3}{2}\binom{n}{2} + \frac{3n-4}{4} - \left[\binom{n}{2} + \frac{2}{n} + 2 - 2(n-1) + (4n+2)\sum_{i \in \mathbb{E}} \frac{1}{i}\right]\end{aligned}$$

$$= \frac{n^2+10n-12}{4} - \frac{2n+2}{n} - (4n+2)\sum_{i\in\mathbb{E}} \frac{1}{i}.$$

If $n = 10$, then

$$\Phi(G) \geq \frac{10^2+10\times 10-12}{4} - \frac{2\times 10+2}{2} - (4\times 10+2)\left(\frac{1}{2}+\frac{1}{4}+\frac{1}{6}+\frac{1}{8}\right) = \frac{1}{2} > 0.$$

If $n \geq 12$, note that

$$\sum_{i\in\mathbb{E}} \frac{1}{i} \leq \frac{n}{24} + \frac{77}{120}.$$

Hence

$$\Phi(G) \geq \frac{5n^2-9n+257}{60} - \frac{2n+2}{n} > 0.$$

The inequality above holds because $5n^3 - 9n^2 - 377n - 120 > 210$ for $n > 10$.

This completes the proof of Lemma 3.3.

Theorem 3.4. *Let G be a connected graph of order $n \geq 9$, having a connected complement $\overline{G}$. Then*

$$\binom{n}{2} + \sum_{j=1}^{n-1} \frac{n-j}{\left\lceil \frac{j}{k} \right\rceil} = \mathbf{H}(P_n^k) + \mathbf{H}\big(\overline{P}_n^k\big) \leq \mathbf{H}(G^k) + \mathbf{H}\big(\overline{G}^k\big) \leq 2\binom{n}{2}.$$

Proof. The upper bound is obvious. In order to demonstrate the validity of the lower bound, we consider the following cases:

Case 1. $\mathrm{diam}(G) = 1$. This is impossible, since in this case $\overline{G}$ is disconnected, which contradicts the assumption.

Case 2. $\mathrm{diam}(G) = 2$. Note that $\mathrm{diam}(\overline{\overline{G}}) = \mathrm{diam}(G) = 2$, then the result can be verified by Corollary 3.2.

Case 3. $\mathrm{diam}(G) = 3$. By Lemma 3.1 (2), there exists a spanning subgraph in $\overline{G}$ which is a double star. This implies that $\mathrm{diam}(\overline{G}) = 2$. If $k = 1$, then by Theorem 1.4, $\mathbf{H}(P_n) + \mathbf{H}(\overline{P}_n) \leq \mathbf{H}(G) + \mathbf{H}(\overline{G})$. If $k = 2$, then by Lemma 3.3, $\mathbf{H}(P_n^2) + \mathbf{H}\big(\overline{P}_n^2\big) \leq \mathbf{H}(G) + \mathbf{H}(\overline{G})$. If $k \geq 3$, then $\mathrm{diam}(G^k) = \mathrm{diam}\big(\overline{G}^k\big) = 1$, and therefore by Corollary 3.2, $\mathbf{H}(G^k) + \mathbf{H}\big(\overline{G}^k\big) = 2\binom{n}{2}$.

Case 4. $\mathrm{diam}(G) > 3$. By Lemma 3.1 (1), it is $\mathrm{diam}(\overline{G}) = 2$. Then by Corollary 3.2, $\mathbf{H}(P_n^k) + \mathbf{H}\big(\overline{P}_n^k\big) \leq \mathbf{H}(G^k) + \mathbf{H}\big(\overline{G}^k\big)$.

With this the proof of Theorem 3.4 is completed. □

Note that the bounds in Theorem 3.4 are the best possible. It is obvious that equality in the lower bound is attained by P_n^k. To see that the upper bound is also the best possible, we construct a sequence of graphs G_n of order n, which is obtained from C_4 by replacing one edge of C_4 by $2K_1 + K_{n-4}$, as depicted in Fig. 2. It is easy to check that $\mathrm{diam}(G_n) = \mathrm{diam}\big(\overline{G}_n\big) = 2$, which implies $\mathrm{diam}(G_n^k) = \mathrm{diam}\big(\overline{G}_n^k\big) = 1$ and $\mathbf{H}(G_n^k) + \mathbf{H}\big(\overline{G}_n^k\big) = 2\binom{n}{2}$.

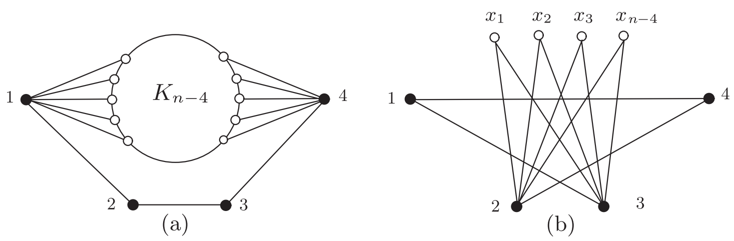

Figure 2. (a) The graph G_n and (b) its complement.

4. CONCLUDING REMARKS

From Theorem 2.2 we know that for any tree T of order n, $\mathbf{H}(P_n) \le \mathbf{H}(T) \le \mathbf{H}(S_n)$ and $\mathbf{H}(P_n^k) \le \mathbf{H}(T^k) \le \mathbf{H}(S_n^k)$. It is natural to ask if the extension of this statement holds for other graphs.

Problem 1. Is it true that for any two graphs G_1 and G_2 of the same order, $\mathbf{H}(G_1) \le \mathbf{H}(G_2)$ implies $\mathbf{H}(G_1^k) \le \mathbf{H}(G_2^k)$?

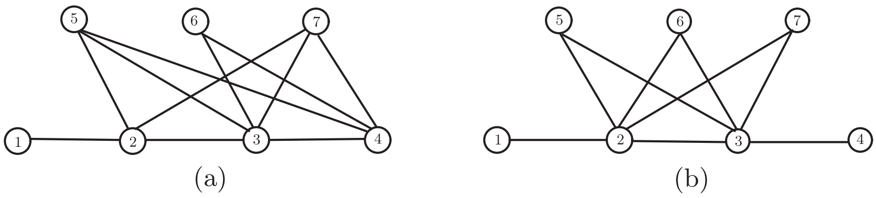

Figure 3. Graphs providing a counterexample for Problem 1.

In fact, the answer is negative. Let G_1 and G_2 be the graphs depicted in Fig. 3 (a) and (b), respectively. Note that $\mathbf{H}(G_1) = 89/6 < \mathbf{H}(G_2) = 94/6$, but $\mathbf{H}(G_1^2) = 41/2 > \mathbf{H}(G_2^2) = 20$.

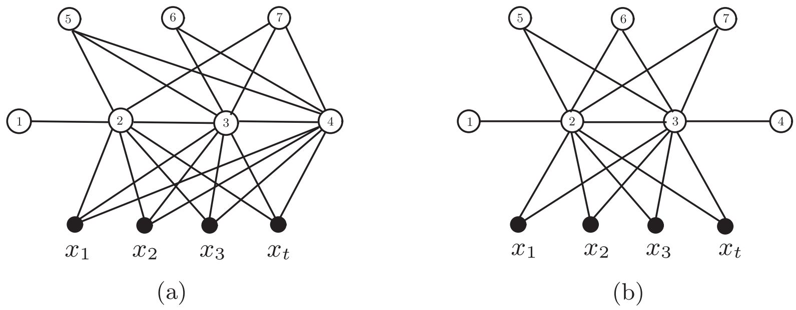

Figure 4. The graphs G_1^* and G_2^*.

It is possible to construct an infinite family of counterexamples of order $n > 7$. Let G_1^* and G_2^* be the graphs depicted in Fig. 4 (a) and (b), respectively. Let G_1^* be obtained from G_1 by adding $t(\geq 2)$ new vertices such that each vertex is only adjacent to vertices 2, 3 and 4 of G_1, cf. Fig. 3. Let G_2^* be obtained from G_2 by adding t new vertices such that each vertex is only adjacent to vertices 2 and 3 of G_2, cf. Fig. 3. Then

$$\mathbf{H}(G_1^*) = \frac{89}{6} + 5t + \frac{1}{2}\binom{t}{2} \qquad \mathbf{H}(G_2^*) = \frac{94}{6} + \frac{9}{2}t + \frac{1}{2}\binom{t}{2}$$
$$\mathbf{H}(G_1^{*,2}) = 20 + 7t + \binom{t}{2} \qquad \mathbf{H}(G_2^{*,2}) = \frac{41}{2} + 7t + \binom{t}{2}.$$

We see that for $t \geq 2$, $\mathbf{H}(G_1^*) > \mathbf{H}(G_2^*)$, but $\mathbf{H}(G_1^{*,2}) < \mathbf{H}(G_2^{*,2})$.

In view of these counterexamples, we propose the following, evidently much more difficult problem.

Problem 2. Characterize the graphs that satisfy the condition in Problem 1.

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