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ON DIAMETER AND INVERSE DEGREE OF CHEMICAL GRAPHS

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The inverse degree $r(G)$ of a finite graph $G = (V, E)$ is defined as $r(G) = \sum_{v \in V} \frac{1}{d(v)}$, where $d(v)$ is the degree of vertex v. In Discrete Math., **310** (2010), 940–946, Mukwembi posed the following conjecture: Let G be a connected chemical graph with diameter diam(G) and inverse degree $r(G)$. Then $\mathrm{diam}(G) \leq \frac{12}{5} r(G) + O(1)$.
In this paper, we settle the conjecture affirmatively.

1. INTRODUCTION

Graph theory terminology not presented here can be found in [**6**]. Let $G = (V, E)$ be a graph with $|V| = n(G)$. The degree, neighborhood and closed neighborhood of a vertex v in the graph G are denoted by $d(v)$, $N(v)$ and $N[v] = N(v) \cup \{v\}$, respectively. The minimum degree and maximum degree of the graph G are denoted by $\delta(G)$ and $\Delta(G)$, respectively. The graph induced by $S \subseteq V$ is denoted by $G[S]$. Let $G - S = G[V - S]$. The graph induced by $E' \subseteq E$ is denoted by $G[E']$. Let $G - E' = G[E - E']$. The distance $d_G(u, v)$ between two vertices u and v of G is the length of the shortest $u - v$ path in G, and the diameter is $\mathrm{diam}(G) = \max\{d_G(u, v) : u, v \in V\}$. The inverse degree $r(G)$ of G is defined as $r(G) = \sum_{v \in V} \frac{1}{d(v)}$. Let P_n, C_n and K_n denote the path, cycle and complete graph with order n, respectively.

Chemical graphs represent the structure of organic molecules and thus have a maximum degree of 4, carbon atoms being 4-valent and double bonds being counted as single edges. Formally, a chemical graph is a graph with a maximum degree of 4.

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The inverse degree (also known as the sum of reciprocals of degrees) first atracted attention through numerous conjectures generated by the computer programme Graffiti [**4**]. Since then its relationship with other graph invariants, such as diameter, edge-connectivity, matching number, Wiener index has been studied by several authors (see, for example [**1**, **2**, **5**]).

Turning to bounds on the diameter in terms of order and inverse degree, our starting point is the following bound by Erdős, Pach and Spencer [**3**].

Theorem 1. *Let G be a connected graph of order n, diameter* $\mathrm{diam}(G)$ *and inverse degree $r(G)$. Then* $\mathrm{diam}(G) \le \big(6r(G) + o(1)\big)\dfrac{\log n}{\log\log n}$.

The bound was later improved by a factor of about 2 by Dankelmann, Swart and van den Berg [**2**], showing that $\mathrm{diam}(G) \le \big(3r(G)+2+o(1)\big)\dfrac{\log n}{\log\log n}$. Mukwembi [**6**] focused on bounds on the diameter in terms of the inverse degree for some important classes of graphs such as planar graphs, regular graph, chemical graphs and trees. Molecular structure-descriptors such as the Randic Index (defined as $R(G) = \sum\limits_{uv\in E(G)} \dfrac{1}{\sqrt{d(u)d(v)}}$), which is similar to that of the inverse degree, were studied intensively for these classes of graphs. Mukwembi [**6**] gave the following result.

Theorem 2. *Let G be a connected chemical graph. Then* $\mathrm{diam}(G) \le 3r(G) + 3$.

In relation to the above theorem, Mukwembi [**6**] conjectured that if G is a connected chemical graph with diameter $\mathrm{diam}(G)$ and inverse degree $r(G)$, then $\mathrm{diam}(G) \le \dfrac{12}{5}r(G) + O(1)$. In this paper, we settle this conjecture affirmatively.

Theorem 3. *Let G be a connected chemical graph with diameter* $\mathrm{diam}(G)$ *and inverse degree $r(G)$. Then* $\mathrm{diam}(G) \le \dfrac{12}{5}r(G)$.

For the upper bound concerning $\mathrm{diam}(G)$, the coefficient $\dfrac{12}{5}$ of $r(G)$ is the best possible. To see this, consider the graph $G = K_1 + K_3 + K_1 + K_1 + K_3 + K_1 + K_1 + K_3 + \ldots + K_1 + K_1 + K_3 + K_1$. Here the operation $A+B$ for two disjoint graphs A, B means joining every vertex of A to every vertex of B with edges completely.

2. PROOF OF THEOREM 3

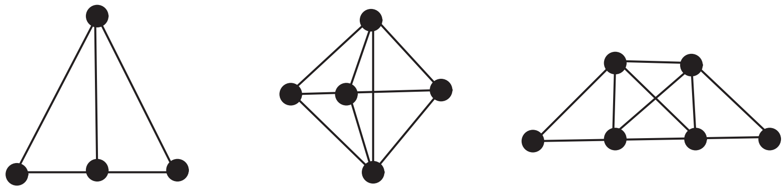
Amongst all connected chemical graphs G, we choose G so that,

(1) $\dfrac{r(G)}{\mathrm{diam}(G)}$ is minimal, and subject to the condition (1),

(2) $n(G)$ is minimal.

In order to prove the theorem, it suffices to show that $\dfrac{r(G)}{\mathrm{diam}(G)} \ge 5/12$. Let $P = v_0v_1\ldots v_{d-1}v_d$ be a diametral path of G. For $i = 0, 1, 2, \ldots, d$, let $N_i =$

$\{v|d(v,v_0)=i\}$. Clearly we have $N_0=\{v_0\}$. If $\mathrm{diam}(G)\le 3$, it is easy to check that $\mathrm{diam}(G)\le \frac{12}{5}r(G)$. Assume that $\mathrm{diam}(G)=4$. Then we have $r(G)\ge \sum_{x\in N[v_0]}\frac{1}{d(x)}+\sum_{x\in N[v_d]}\frac{1}{d(x)}\ge 2$, and so $\mathrm{diam}(G)\le \frac{12}{5}r(G)$. Also notice that, if $6\ge \mathrm{diam}(G)\ge 5$, then $r(G)\ge \sum_{x\in N[v_0]}\frac{1}{d(x)}+\frac{1}{d(v_2)}+\frac{1}{d(v_3)}+\sum_{x\in N[v_d]}\frac{1}{d(x)}\ge 5/2$, meaning that $\mathrm{diam}(G)\le \frac{12}{5}r(G)$ holds. Hence, in the following argument, we may assume that $\mathrm{diam}(G)\ge 7$. For $i=0,1,2,\dots,d$, let $S_i=\{v|v\in N_i, d(v)<4\}$. We define some graphs which will play an important role in the proof of our main result.



F_1 F_2 F_3

Claim 1. *The following statements hold*:

(i) $\delta(G)\ge 2$.

(ii) *For every* $1\le i\le d-1$, $G[S_i\cup S_{i+1}]$ *forms a complete graph. In particular, for any* $v\in S_i$ *and* $u\in N_{i-1}\cup N_i\cup N_{i+1}$, *if* $vu\notin E(G)$ *then* $d(u)=4$.

(iii) *For every* $1\le i\le d-1$, $|S_{i-1}\cup S_i\cup S_{i+1}|\le 3$.

(iv) *Let* v *be a vertex with* $d(v)=2$ *such that* $v\in N_i$ *for some* $1\le i\le d-1$. *Then, for any edge* $e=ab$ *with* $N(v)\cap\{a,b\}=\emptyset$, $|(N_{i-1}\cup N_i\cup N_{i+1})\cap\{a,b\}|\le 1$.

Proof. To prove (i), suppose that there exists a vertex $v\in V(G)$ such that $d(v)=1$. Then $v\in (V(G)-V(P))\cup\{v_0,v_d\}$. Since P is a diametral path, it follows that $v\notin N_1$. If $v\in V(G)-V(P)$, let u be the neighbour of v and $G'=G-\{v\}$. Then $\mathrm{diam}(G')\ge d$. Moreover, $d_{G'}(x)=d_G(x)$ for all $x\notin\{u,v\}$. Since $d(u)\ge 2$, we have $r(G)-r(G')=\frac{1}{d(v)}+\frac{1}{d(u)}-\frac{1}{d(u)-1}=1+\frac{1}{d(u)}-\frac{1}{d(u)-1}>0$. Then $\frac{r(G)}{\mathrm{diam}(G)}-\frac{r(G')}{\mathrm{diam}(G')}>0$, which is a contradiction. If $d(v_0)=1$, let G' be obtained from G and K_3 by joining edges from v_0 to each vertex of K_3. Then $\mathrm{diam}(G')=d+1$. Moreover, $d_{G'}(v)=d_G(v)$ for all $v\in V(G)-\{v_0\}$. Let $x=\sum_{v\in V(G)-\{v_0\}}\frac{1}{d(v)}$. Then $x\ge \frac{d}{4}$, $r(G)=x+1$ and $r(G')=x+\frac{5}{4}$. So, $\frac{r(G)}{\mathrm{diam}(G)}-\frac{r(G')}{\mathrm{diam}(G')}=\frac{x+1}{d}-\frac{x+\frac{5}{4}}{d+1}>0$, which is a contradiction. Hence, $d(v_0)\ge$

2. Similarly, $d(v_d) \geq 2$. So, $\delta(G) \geq 2$. Thus (i) holds. Next suppose that there exist two vertices $u, v \in S_i \cup S_{i+1}$ such that $uv \notin E(G)$. Let $G' = G \cup \{uv\}$. Note that $\mathrm{diam}(G) = \mathrm{diam}(G')$. Since $r(G) - r(G') = \frac{1}{d(u)} + \frac{1}{d(v)} - \frac{1}{d(u)+1} - \frac{1}{d(v)+1} > 0$, $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, which is a contradiction. Thus (ii) holds. To prove (iii), suppose $|S_{i-1} \cup S_i \cup S_{i+1}| \geq 4$ and take $u_1, u_2, u_3, u_4 \in S_{i-1} \cup S_i \cup S_{i+1}$. Let G' be the graph obtained from G by adding a new vertex v to N_i with edges u_1v, u_2v, u_3v, u_4v (i.e., $G' = G \cup \{v\} \cup \{u_1v, u_2v, u_3v, u_4v\}$). Then one can easily check that $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, a contradiction. Thus (iii) holds.

To show (iv), suppose that $a, b \in N_{i-1} \cup N_i \cup N_{i+1}$ where $ab \in E(G)$, $v \in N_i$ and $d(v) = 2$. Consider the graph $G' = (G - \{ab\}) \cup \{av, bv\}$. Then we have $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, a contradiction. Thus (iv) holds.

Claim 2. *If there exists a vertex $v \in N_i$ such that $d(v) = 2$, then $N_i = \{v\} = \{v_i\}$.*

Proof. Since $N_0 = \{v_0\}$, we can assume that $v \in N_i$, where $i \in \{1, 2, \ldots, d\}$. Let $u \in N(v) \cap N_{i-1}$. Suppose that $N_i - \{v\} \neq \emptyset$. For any $w \in N_i - \{v\}$, if $wv \notin E(G)$, then $d(w) = 4$. Then there exists a vertex $t \in N(w) - N(v)$ such that $vt \notin E(G)$. Since $N(v) \cap \{w, t\} = \emptyset$, we get a contradiction to Claim 1(iv). Hence, $wv \in E(G)$ for any $w \in N_i - \{v\}$. Since $d(v) = 2$, $N_i = \{v, w\}$. Furthermore, $uw \in E(G)$. Otherwise, let $G' = (G - \{v\}) \cup \{uw\}$. Then $\mathrm{diam}(G') = d$ and $r(G) - r(G') > 0$. So, $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, which is a contradiction. Since $\mathrm{diam}(G) \geq 7$, $d(u) \geq 3$ or $d(w) \geq 3$. If $d(u) \geq 3$ and $d(w) \geq 3$, let $G' = G - \{v\}$. Then $\mathrm{diam}(G') = d$ and $r(G) - r(G') > 0$. So, $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, which is a contradiction. If $d(u) = 2$ and $d(w) \geq 3$, then $N_0 = \{u\}$. Let G' be obtained from G by adding a vertex ℓ and joining edges ℓu and ℓv. Then $\mathrm{diam}(G') = d + 1$. Let $x = \sum_{z \in V(G) - \{u,v\}} \frac{1}{d(z)}$. Then $x \geq \frac{d}{4}$, $r(G) = x + 1$ and $r(G') = x + \frac{7}{6}$. So, $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} = \frac{x+1}{d} - \frac{x + \frac{7}{6}}{d+1} > 0$, which is a contradiction. If $d(u) \geq 3$ and $d(w) = 2$, then $N_d = \{v, w\}$. In a similar way as above, there is a contradiction. So $N_i = \{v\} = \{v_i\}$.

Claim 3. *For $i \in \{2, 3, \ldots, d-2\}$, if there exists a vertex $v \in N_i - \{v_i\}$ such that $d(v) = 4$, say $N(v) = \{u, w, t, s\}$, then the following statements hold:*

(1) *Suppose that $uw \notin E(G)$. If $u, w \in N_{i-1} \cup N_i$ or $u, w \in N_i \cup N_{i+1}$, then $d(t) = d(s) = 3$ holds.*

(2) $N(v) \cap N_{i+1} \neq \emptyset$.

Proof. Since $v \notin V(P)$ and $2 \leq i \leq d-2$, in view of Claim 2, $d(u), d(w), d(t), d(s) \geq 3$. Furthermore, there exists a vertex of degree 4 in $N(v)$.

(1) If $u, w \in N_{i-1} \cup N_i$ or $u, w \in N_i \cup N_{i+1}$, then $d(t) = d(s) = 3$. Otherwise, let $G' = (G - \{v\}) \cup \{uw\}$. Then $\mathrm{diam}(G') \geq d$. Since $r(G) - r(G') \geq 0$, $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} \geq 0$ and $n(G') < n(G)$, which is a contradiction.

(2) Suppose that $N(v) \subseteq N_{i-1} \cup N_i$. Then $N[v] \cong K_5$. Otherwise, say $uw \notin E(G)$. Then $d(s) = d(t) = 3$ and $st \in E(G)$. Since $sw \notin E(G)$ or $su \notin E(G)$, we can assume that $sw \notin E(G)$. Then $d(u) = d(t) = 3$ and $ut, us \in E(G)$. Since $i \geq 2$, $\{u, s, t\} \cap N_{i-1} = \emptyset$. Hence, $\{u, s, t\} \subseteq N_i$. Then $N(u) \cap N_{i-1} = \emptyset$, which is a contradiction. Since $N[v] \cong K_5$, $G \cong K_5$, which is a contradiction. So, $N(v) \cap N_{i+1} \neq \emptyset$.

Claim 4. *For $i \in \{2, 3, \cdots, d-2\}$, if there exists a vertex $v \in N_i - \{v_i\}$ such that $d(v) = 3$, then $G[N_{i-1} \cup N_i \cup N_{i+1}] \cong F_1$.*

Proof. Let $N(v) = \{u, w, t\}$. Since $v \notin V(P)$ and $2 \leq i \leq d-2$, Claim 2 implies $d(u), d(w), d(t) \geq 3$. First we observe that for any $x, y \in N(v)$, if $x, y \in N_{i-1} \cup N_i$ or $x, y \in N_i \cup N_{i+1}$ then $xy \in E(G)$. To see this, suppose $xy \notin E(G)$, and let $G' = (G - \{v\}) \cup \{xy\}$. Then $\mathrm{diam}(G') \geq d$. Since $r(G) - r(G') > 0$, we have $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, which is a contradiction.

Since $|S_{i-1} \cup S_i \cup S_{i+1}| \leq 3$ by Claim 1(iii), at least one vertex of $N(v)$ has degree 4. Suppose that $d(u) = 4$. Then $d(w) = d(t) = 3$. Otherwise, let $G' = G - \{v\}$. Then $\mathrm{diam}(G') \geq d$. Since $r(G) - r(G') \geq 0$, we have $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} \geq 0$ and $n(G') < n(G)$, which is a contradiction. If $N(v) \subseteq N_{i-1} \cup N_i$, then $G[N[v]] \cong K_4$ by the above observation. So, $u \in N_{i-1}$ and $\{w, t\} \subseteq N_i$ (because $2 \leq i$ and $d(w) = d(t) = 3$). Since $i \leq d-2$, we have $v, w, t \notin V(P)$. So $u \notin V(P)$. Let $G' = G - N[v]$. Then $\mathrm{diam}(G') \geq d$. Since $r(G) - r(G') > 0$, $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, which is a contradiction. Hence, $N(v) \cap N_{i-1} \neq \emptyset$.

Case 1. $|N(v) \cap N_{i-1}| = 2$.

Without loss of generality, we can assume that $w \in N_{i-1}$. Since $N(w) \cap N_{i-2} \neq \emptyset$, it follows that $wv_i \notin E(G)$. If there exists a vertex $s \in N(v_i) \cap (N_{i-1} \cup N_i) - N(v) \cap N_{i-1}$, let $G' = (G - \{v_i s\}) \cup \{v_i w, vs\}$. Then $\mathrm{diam}(G') \geq d$. Since $r(G) - r(G') > 0$, we have $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, which is a contradiction. Hence, $N(v_i) \cap (N_{i-1} \cup N_i) - N(v) \cap N_{i-1} = \emptyset$. That is $N(v) \cap N_{i-1} = \{w, u\}$, $uv_i \in E(G)$ and $|N(v_i) \cap N_{i+1}| \geq 3$. Since $d(t) = 3$, there exists a vertex $s \in N(v_i) \cap N_{i+1}$ such that $ts \notin E(G)$. Let $G' = (G - \{v_i s\}) \cup \{v_i v, ts\}$. Then $\mathrm{diam}(G') \geq d$. Since $r(G) - r(G') > 0$, we have $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, which is a contradiction.

Case 2. $|N(v) \cap N_{i-1}| = 1$ and $|N(v) \cap N_i| = 1$.

Without loss of generality, we can assume that $w \in N(v) \cap (N_{i-1} \cup N_i)$. If $|N_i| > 2$, say $s \in N_i - N[v]$. By the above observation, $sw \notin E(G)$. Note that, by Claim 1(ii), $d(s) = 4$. Let $k \in N(s) - N(v)$ and $G' = (G - \{sk\}) \cup \{sw, kv\}$.

Then $\operatorname{diam}(G') \geq d$. Since $r(G) - r(G') > 0$, we have $\frac{r(G)}{\operatorname{diam}(G)} - \frac{r(G')}{\operatorname{diam}(G')} > 0$, which is a contradiction. Hence, $|N_i| = 2$. That is $N_i = \{v, v_i\}$ and $vv_i \in E(G)$. If $d(v_i) = 4$, then $v_i = u$, $w \in N_{i-1}$ and $t \in N_{i+1}$. Let $s \in N(v_i) - N(v)$ and $k \in N(s) - N(w) \cup N(t)$. Let $G' = (G - \{sk\}) \cup \{kw, sv\}$ or $G' = (G - \{sk\}) \cup \{kt, sv\}$. Then $\operatorname{diam}(G') \geq d$. Since $r(G) - r(G') > 0$, we have $\frac{r(G)}{\operatorname{diam}(G)} - \frac{r(G')}{\operatorname{diam}(G')} > 0$, which is a contradiction. Hence $d(v_i) = 3$. That is $w = v_i$. Then $|N_{i+1}| = 1$. If $|N_{i-1}| \geq 2$, let $s \in N_{i-1} - N(v)$, then $d(s) = 4$ and $N(s) \cap N_i = \emptyset$. If $i \geq 3$, by Claim 3, there is a contradiction. If $i = 2$, then $|N_0 \cup N_1| \geq 6$, there is a contradiction. Hence $|N_{i-1}| = 1$. So $G[N_{i-1} \cup N_i \cup N_{i+1}] \cong F_1$.

Case 3. $|N(v) \cap N_{i-1}| = 1$ and $|N(v) \cap N_{i+1}| = 2$.

We may assume that $t \in N(v) \cap N_{i+1}$. Then $v_i t \notin E(G)$. Otherwise, let $G' = (G - \{t\}) \cup \{vv_i\}$. Then $\operatorname{diam}(G') \geq d$. Since $r(G) - r(G') > 0$, we have $\frac{r(G)}{\operatorname{diam}(G)} - \frac{r(G')}{\operatorname{diam}(G')} > 0$, which is a contradiction. In a similar way as Case 1, it follows that $N(v_i) \cap (N_i \cup N_{i+1}) = \{u\}$. That is $w \in N_{i-1}$ and $|N(v_i) \cap N_{i-1}| = 3$. In a similar way as Case 1, there is a contradiction.

Claim 5. *For $i \in \{3, 4, \ldots, d-3\}$, if there exists a vertex $v \in N_i - \{v_i\}$ such that $d(v) = 4$, then one of the following statements hold:*

(1) $G[N_{i-1} \cup N_i \cup N_{i+1}] \cong F_2$.

(2) $G[N_{i-1} \cup N_i \cup N_{i+1} \cup N_{i+2}] \cong F_3$.

(3) $G[N_{i-2} \cup N_{i-1} \cup N_i \cup N_{i+1}] \cong F_3$.

Proof. Let $N(v) = \{u, w, t, s\}$. By Claim 3, $N(v) \cap N_{i+1} \neq \emptyset$.

Case 1. $|N(v) \cap N_{i-1}| = 3$ and $|N(v) \cap N_{i+1}| = 1$.

We may assume that $u, w, t \in N_{i-1}$ and $s \in N_{i+1}$. If $G[\{u, w, t\}] \cong K_3$, then $d(u) = d(w) = d(t) = 4$. Let $\ell \in N(u) \cap N_{i-2}$. Since $u \neq v_{i-1}$, applying Claim 3(1) to u, we also have $\ell \in N(w) \cap N(t)$. Let $G' = G - \{v, w, u, t\}$. Since $u, w, t \notin V(P)$ and $d(s) \geq 3$, $\operatorname{diam}(G') \geq d$ and $r(G) - r(G') > 0$. So, $\frac{r(G)}{\operatorname{diam}(G)} - \frac{r(G')}{\operatorname{diam}(G')} > 0$, which is a contradiction. Without loss of generality, we can assume that $uw \notin E(G)$. Then, in view of Claim 3(1), we have $d(t) = d(s) = 3$. Since $ut \notin E(G)$ or $wt \notin E(G)$, say $ut \notin E(G)$, then $d(w) = 3$ and $wt \in E(G)$. Hence $w \neq v_{i-1}$. By Claim 4, there is a contradiction.

Case 2. $|N(v) \cap N_{i-1}| = 2$ and $|N(v) \cap N_i| = 1$.

We may assume that $u, w \in N_{i-1}$, $t \in N_i$ and $s \in N_{i+1}$. Suppose that $G[\{u, w, t\}] \cong K_3$. Since $d(u) = d(w) = 4$, in view of Claim 3, we must have $st \in E(G)$. Without loss of generality, assume $u \notin V(P)$. Let $\ell \in N(u) \cap N_{i-2}$. By Claim 3, we have $\ell w \in E(G)$.

If there exists a vertex $h \in N_i - \{v, t\}$, let $h_1 \in N(h) \cap N_{i-1}$ and $G' = (G - \{v\} - \{hh_1\}) \cup \{th_1, wh\}$. Then $\frac{r(G)}{\operatorname{diam}(G)} - \frac{r(G')}{\operatorname{diam}(G')} \geq 0$ and $n(G') < n(G)$, which is a contradiction. Hence $N_i = \{v, t\}$. Since $N_i = \{v, t\}$, $N_{i+1} = \{s\}$. Suppose that there exists a vertex $h \in N_{i-1} - \{u, w\}$. Since $h \neq v_{i-1}$, by Claim 4, $d(h) = 4$. Since $N(h) \cap N_i = \emptyset$, by Claim 3, there is a contradiction. Hence, $N_{i-1} = \{u, w\} = \{u, v_{i-1}\}$. Arguing similarly as above, we can prove that $N_{i-2} = \{l\}$. So, $G[N_{i-2} \cup N_{i-1} \cup N_i \cup N_{i+1}] \cong F_3$.

Assume for the moment that $uw \notin E(G)$. By Claim 3, $d(t) = d(s) = 3$ and hence $st \in E(G)$ by Claim 1(ii). Since $ut \notin E(G)$ or $wt \notin E(G)$, say $ut \notin E(G)$, then $d(w) = 3$ and $wt \in E(G)$. Since $v \notin V(P)$, by Claim 4, $t = v_i$, $w = v_{i-1}$ and $s = v_{i+1}$. Since $d(u) = 4$ by Claim 1(iii), there exists a vertex $f \in N(u) - N(w)$. Let $G' = (G - \{uf\}) \cup \{ut, wf\}$. Then $\mathrm{diam}(G') \geq d$ and $r(G) - r(G') > 0$. So, $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, which is a contradiction.

Hence $uw \in E(G)$. Without loss of generality, we can assume that $ut \notin E(G)$. Then $d(w) = d(s) = 3$. It is easy to check that $w \notin V(P)$. Then, applying Claim 4 to w, we get a contradiction.

Case 3. $|N(v) \cap N_{i-1}| = 1$ and $|N(v) \cap N_i| = 1$.

We may assume that $u \in N_{i-1}$, $w \in N_i$ and $s, t \in N_{i+1}$. Suppose that $G[\{w, s, t\}] \cong K_3$. If $d(s) = 3$, let $G' = G - \{s\}$. Then $\mathrm{diam}(G') \geq d$. Since $r(G) - r(G') \geq 0$, $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} \geq 0$ and $n(G') < n(G)$, which is a contradiction. Hence, $d(s) = 4$. Similarly, $d(t) = 4$. Then $uw \in E(G)$ by Claim 3(1). Say $s \neq v_{i+1}$. Let $\ell \in N(s) - \{v, w, t\}$. By Claim 3, $\ell \in N_{i+2}$ and $t\ell \in E(G)$. By a similar proof as Case 2, $G[N_{i-1} \cup N_i \cup N_{i+1} \cup N_{i+2}] \cong F_3$.

Assume that $st \notin E(G)$. Then $d(u) = d(w) = 3$. Since $wt \notin E(G)$ or $ws \notin E(G)$, say $ws \notin E(G)$, then $d(t) = 3$ and $wt \in E(G)$. By Claim 4, $w = v_i$, $u = v_{i-1}$, $t = v_{i+1}$. By Claim 1, $d(s) = 4$. Then there exists a vertex $f \in N(s) - N(t)$, let $G' = (G - \{sf\}) \cup \{sw, ft\}$. Then $\mathrm{diam}(G') \geq d$ and $r(G) - r(G') > 0$. So, $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, which is a contradiction. Hence $st \in E(G)$. Without loss of generality, we can assume that $sw \notin E(G)$. Then $d(u) = d(t) = 3$. By Claim 4, $t = v_{i+1}$. Hence $v = v_i$, which is a contradiction.

Case 4. $|N(v) \cap N_{i-1}| = 1$ and $|N(v) \cap N_{i+1}| = 3$.

We may assume that $u \in N_{i-1}$ and $w, s, t \in N_{i+1}$. Assume for the moment that $G[\{w, s, t\}] \cong K_3$. Since $i \leq d - 3$, if there exists a vertex $x \in \{w, s, t\}$ such that $d(x) = 3$, then $x \neq v_{i+1}$. But one can easily see that this structure contradicts Claim 4. So we have $d(w) = d(s) = d(t) = 4$. Since $G[\{w, s, t\}] \cong K_3$ and $v \neq v_i$, it is easy to check that $\{w, s, t\} \cap \{v_{i+1}\} = \emptyset$. By Claim 3, there exists a vertex $y \in N_{i+2}$ such that $\{w, s, t\} \subset N(y)$. Let $G' = G - \{v, w, s, t, y\}$. Then we get $\mathrm{diam}(G') \geq d$. Also, since $d(u) \geq 3$ and $i \leq d - 3$, it is easy to check that $r(G) - r(G') > 0$. So we have $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, a contradiction.

Hence, without loss of generality, we may assume that $ws \notin E(G)$. Then we have $d(u) = d(t) = 3$ by Claim 3. Since $d(w) = 4$ or $d(s) = 4$, we can assume that $d(w) = 4$. Then $st \in E(G)$. Since $i \leq d - 3$ and $d(t) = 3$, we have $t \notin V(P)$. Applying Claim 4 to t, we can easily get a contradiction.

Case 5. $|N(v) \cap N_{i-1}| = 1$, $|N(v) \cap N_i| = 2$ and $|N(v) \cap N_{i+1}| = 1$.

We may assume that $u \in N_{i-1}$, $w, t \in N_i$ and $s \in N_{i+1}$. Suppose that $G[\{u, w, t\}] \cong K_3$. Then we have $d(u) = 4$. By Claim 3, $ws, ts \in E(G)$. If $u \notin V(P)$, let $G' = (G - \{t\} - \{v_{i-1}v_i\}) \cup \{uv_i, v_{i-1}v\}$. Then $\mathrm{diam}(G') \geq d$ and $r(G) - r(G') \geq 0$. So $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} \geq 0$ and $n(G') < n(G)$, which is a contradiction. Hence, $u = v_{i-1}$. Suppose there exists a vertex $l \in N_{i-1} - \{u\}$. Then there exists a vertex $f \in N(\ell) - N_u$ such that $\ell f \in E(G)$. Then, letting $G' = (G - \{v\} - \{\ell f\}) \cup \{fu, w\ell\}$, we get $\mathrm{diam}(G') \geq d$ and $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, a contradiction. Hence $N_{i-1} = \{u\}$ and this implies $G[N_{i-1} \cup N_i \cup N_{i+1}] \cong F_2$, as desired.

Thus we may assume that $uw \notin E(G)$. By Claim 3, $d(t) = d(s) = 3$. Hence by Claim 1(ii), $st \in E(G)$. Since $t \in N_i$, we have $N(t) \cap N_{i-1} \neq \emptyset$. This implies $wt \notin E(G)$. Then by Claim 3, $d(u) = 3$ and $ut \in E(G)$. Hence $d(w) = 4$ (by Claim 1(ii)). Since $v \notin V(P)$, by Claim 4, $t = v_i$, $u = v_{i-1}$ and $s = v_{i+1}$. Let f be a vertex with $wf \in E(G)$ and $f \neq v$. Let $G' = (G - \{wf\}) \cup \{uw, ft\}$. Then we have $\mathrm{diam}(G') \geq d$ and $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, a contradiction. Hence $uw \in E(G)$. We can similarly have $ut \in E(G)$. Since $G[\{u, w, t\}] \not\cong K_3$, $wt \notin E(G)$. So, $d(u) = 3$. Then $N(u) \cap N_{i-2} = \emptyset$, which is a contradiction.

Case 6. $|N(v) \cap N_{i-1}| = 2$ and $|N(v) \cap N_{i+1}| = 2$.

We may assume that $u, w \in N_{i-1}$ and $s, t \in N_{i+1}$. It is easy to check that $uw \in E(G)$ or $st \in E(G)$ holds. (Otherwise, let $G' = (G - \{v\}) \cup \{uw, st\}$. Then $\mathrm{diam}(G') \geq d$ and $r(G) - r(G') > 0$. So $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, which is a contradiction.) Suppose that $uw \in E(G)$ and $st \notin E(G)$. By Claim 3, $d(u) = d(w) = 3$. This together with $v \notin V(P)$ implies $u, w \notin V(P)$. Then, applying Claim 4 to u, we get a contradiction. We can similarly get a contradiction in the case where $uw \notin E(G)$ and $st \in E(G)$.

Hence we may assume that $uw \in E(G)$ and $st \in E(G)$. If $d(u) = d(w) = 3$ or $d(s) = d(t) = 3$, in view of Claim 4, we get a contradiction. Hence, without loss of generality, we may assume that $d(u) = d(s) = 4$. Let $N(s) - \{v, t\} = \{s_1, s_2\}$ and $N(u) - \{v, w\} = \{u_1, u_2\}$.

Assume for a while that $s \notin V(P)$. Applying Claim 3 to s, we may assume that $s_1 \in N_{i+2}$. If $s_2 \in N_i \cup N_{i+1}$, then by Claim 3, we have $d(t) = d(s_1) = 3$. In this case, applying Claim 4 to t, we can easily get a contradiction. Thus we have $\{s_1, s_2\} \subset N_{i+2}$. Applying Claim 3 to s, $G[\{s_1, s_2, v, s\}] = K_4$. Furthermore, it is easy to prove that $d(s_1) = d(s_2) = 4$.

If $G - v$ is connected, then let $G' = G - \{v, s, t\}$. If $G - v$ is disconnected, then there is a connected component C such that $V(C) \supset \{s, t, s_1, s_2\}$ and $G - C$ is connected. In this case, let $G' = G - C$. In any case, since G' is connected and $\mathrm{diam}(G') \geq d$, we get a contradiction to the choice of G.

Finally assume that $s \in V(P)$. We may assume that $s_1 = v_{i+2}, s_2 = v_i$. In view of Claim 4, we have $d(t) = 4$. In view of Claim 3, we have $s_1t, s_2t \in E(G)$ because $d(v) = 4$. Since $vs_2 \notin E(G)$, applying Claim 3 to t, we get a contradiction because $d(s) = 4$.

Claim 6. *For every* $2 \le i \le d-2$, $N_{i-1} \cup N_i \cup N_{i+1}$ *contains a vertex of degree at least* 3.

Proof. Assume the opposite. Then by Claim 2, we have $d(v_{i-1}) = d(v_i) = d(v_{i+1}) = 2$ for some i. Let G' be a graph obtained from G by adding a new vertex u such that $uv_{i-1}, uv_i, uv_{i+1} \in E(G')$. Then we can easily check that $\frac{r(G)}{\mathrm{diam}(G)} - \frac{r(G')}{\mathrm{diam}(G')} > 0$, which contradicts the choice of G. □

Now we find a block decomposition of G. Notice that, in view of Claims 2, 4, 5, G has a cut vertex. So there exist at least two blocks. Let $\mathcal{B}_0$ be a set of blocks such that each $B \in \mathcal{B}_0$ is isomorphic to K_2 and B contains a vertex v_j with $d(v_j) = 2$ for some $3 \le j \le d-2$. Moreover, let $\mathcal{B}_0^1 = \{B \in \mathcal{B}_0 | V(B) = \{v_{i-1}, v_i\}$ for some $3 \le i \le d-2$ such that $N_i = \{v_i\}, d(v_{i-1}) > 2, d(v_i) = 2$ and $d(v_{i+1}) > 2\}$ and $\mathcal{B}_0^2 = \{B \in \mathcal{B}_0 | V(B) = \{v_i, v_{i+1}\}$ for some $2 \le i \le d-2$ such that $N_i = \{v_i\}, N_{i+1} = \{v_{i+1}\}, d(v_i) = d(v_{i+1}) = 2\}$.

For $i = 1, 2, 3$, let $\mathcal{B}_i$ be a set of blocks such that each $B \in \mathcal{B}_i$ is isomorphic to F_i and $V(B) \cap \{v_2, v_3, \ldots, v_{d-2}\} \ne \emptyset$. Let $\mathcal{B} = \mathcal{B}_0^1 \cup \mathcal{B}_0^2 \cup (\bigcup_{i=1}^3 \mathcal{B}_i)$. Also, for each $1 \le i \le 3$, put $b_i = |\mathcal{B}_i|$, and for $j = 1, 2$, put $b_{0j} = |\mathcal{B}_0^j|$. For a pair of blocks $B, B' \in \mathcal{B}_1 \cup \mathcal{B}_3$, it is possible that B and B' share exactly one vertex (i.e., it is a cut vertex of G). Let x be the number of such pairs in $\mathcal{B}_1 \cup \mathcal{B}_3$. Also let $Y = V(P) - \cup_{B \in \mathcal{B}} V(B)$ and $y = |Y|$. Note that, in view of Claims 2-6, $Y \subset \{v_0, v_1, v_2, v_3, v_{d-3}, v_{d-2}, v_{d-1}, v_d\}$. Put $I = \{i | v_i \in Y\}$ and $M = \{v \in V(G) | v \in N_i$ for some $i \in I\}$.

Claim 7. *The following statements hold*:

(i) *For* $i \le 3$, *if* $v_i \in Y$, *then* $v_j \in Y$ *for each* j *with* $j < i$. *Similarly, for* $i \ge d-3$, *if* $v_i \in Y$, *then* $v_j \in Y$ *for each* j *with* $i < j$.

(ii) *If* $v_3 \in Y$, *then* $\sum_{v \in N_2 \cup N_3} \frac{1}{d(v)} \ge \frac{5}{6}$. *Similarly, if* $v_{d-3} \in Y$, *then* $\sum_{v \in N_{d-2} \cup N_{d-3}} \frac{1}{d(v)} \ge \frac{5}{6}$.

(iii) $\sum_{v \in M} \frac{1}{d(v)} \ge 5y/12$.

Proof. We can easily see that, if $v_i \in Y$ holds for $i \le 2$ or $i \ge d-2$, then the assertion of (i) follows from the structure of F_i for $1 \le i \le 3$ and $\delta(G) \ge 2$ by Claim 1(i). Suppose that $v_3 \in Y$. If $|N(v_3) \cap N_2| \ge 2$, then we can easily check that $\{v_0, v_1, v_2\} \subset Y$. So we may assume that $N(v_3) \cap N_2 = \{v_2\}$. If $d(v_3) = 2$, then $\{v_2, v_3\}$ forms a block in $\mathcal{B}_0^1 \cup \mathcal{B}_0^2$, which contradicts $v_3 \in Y$. So we have $d(v_3) \ge 3$. Then, applying Claim 4 or 5 to a vertex of $N(v_3) - V(P)$, we find a block $B \in \cup_{1 \le i \le 3} \mathcal{B}_i$ containing v_3, a contradiction. For the case where $v_{d-3} \in Y$, the almost identical argument works. Thus (i) holds.

To show (ii), suppose that $v_3 \in Y$. In view of Claims 2, 4, 5, this forces $|N(v_3) \cap N_2| \geq 2, N_3 = \{v_3\}$ and $N(v_3) \cap N_4 = \{v_4\}$ (otherwise, v_3 is contained in a block of $\mathcal{B}$). Since $d(v_3) \geq 3$ and $\Delta(G) \leq 4$, we have $\sum_{v \in N_2 \cup N_3} \frac{1}{d(v)} \geq 5/6$. For the case $v_{d-3} \in Y$, the almost identical argument works. To show (iii), by (i) it suffices to show that, for any maximal subset L of I such that $L = \{0, 1, \ldots, \ell\}$ or $L = \{d, d-1, \ldots, d-\ell\}$ and $Z = \cup_{i \in L} V(N_i)$, $\sum_{z \in Z} \frac{1}{d(z)} \geq 5|L|/12$. Note that if $I \neq \emptyset$ then $1 \leq |L| \leq 4$ by the definition of Y and I. By the Claims 2, 4, 5, $2 \leq |L| \leq 4$. Since the argument of the proof is almost identical, we only discuss the case where $L = \{0, 1, \ldots, \ell\}$. If $|L| = 2$, then $\sum_{z \in Z} \frac{1}{d(z)} \geq \sum_{x \in N[v_0]} \frac{1}{d(x)} \geq 1 > 5/6$, as claimed. If $|L| = 3$, in view of Claim 2, it is easy to see that $d(v_1) \geq 3$. Then we have $\sum_{z \in Z} \frac{1}{d(z)} \geq \max\left\{ \sum_{x \in N[v_0]} \frac{1}{d(x)}, \sum_{x \in N[v_1]} \frac{1}{d(x)} \right\} \geq 5/4$, as claimed. If $|L| = 4$, then by (ii), $\sum_{v \in M} \frac{1}{d(v)} \geq \sum_{x \in N[v_0]} \frac{1}{d(x)} + \sum_{v \in N_2 \cup N_3} \frac{1}{d(v)} \geq 1 + 5/6 > 5/3$, as claimed. □

Now we construct a graph G^* from G as follows: For every pair of blocks $B, B' \in \mathcal{B}_1 \cup \mathcal{B}_3$ sharing one cut vertex v (i.e., $|B \cap B'| = 1$), delete v and add two new vertices v', v'' with an edge $e = v'v''$ and join v' to $N(v) \cap B$ completely, v'' to $N(v) \cap B'$ completely with edges (i.e., this operation corresponds to replacing a cutvertex by a bridge). Let G^* be the resulting graph. By this construction, we have $d(G^*) = d + x$.

Then, in view of Claims 2-5 and 7(iii), we get that $r(G^*) = r(G) + 5x/12 \geq b_{01}/2 + b_{02} + 4b_1/3 + 5b_2/4 + 5b_3/3 + 5y/12$ and $d(G^*) = d + x \leq b_{01} + 2b_{02} + 3b_1 + 3b_2 + 4b_3 + y$.

Consequently we have $d \leq \frac{12}{5} r(G)$, as desired. This completes the proof of Theorem 3.

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