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Tricyclic Graphs with Minimum Values of PI Index*

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Abstract

In this paper, we give the lower bound on the PI index of connected tricyclic graphs and characterize the graphs with minimum PI index.

1 Introduction and background

Let $G = (V, E)$ be a simple connected graph with $n = |V|$ vertices and $m = |E|$ edges. For more notations and terminologies that will be used, see [6]. For each edge $e = (u, v) \in E$, let $m_u(e|G)$ be the number of edges in G lying closer to vertex u than to the vertex v, and similarly, let $m_v(e|G)$ be the number of edges in G lying closer to vertex v than to the vertex u. The Padmakar-Ivan index, abbreviated as PI index, is defined as

$$PI(G) = \sum_{e=(u,v)\in E} [m_u(e|G) + m_v(e|G)]$$

The Padmakar-Ivan index was first introduced in [17]. Its discriminating power in QSPR/QSAR studies was discussed in [17], while its basic mathematical properties have been considered in [4]. The values of PI index for a number of classes of molecular graphs have been obtained in [1–3, 5, 7, 10–13, 15, 21, 22]. The computation of the PI index in

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partial cubes and benzenoids has been studied in [14, 19], for product graphs it has been obtained in [24], while for bridge and chain graphs it has been given in [23]. A survey of a number of other results and applications of PI index is given in [16].

Another questions that attracted attention of researchers are the bounds and the extremal graphs for PI index. It has been shown by Deng [8] that $PI(G) \geq M_1(G) - 2m$ with equality if and only if G is a complete multipartite graph, where $M_1(G)$ is the sum of the squares of the vertex degrees of G, usually referred to as the first Zagreb index of G. Deng [9] show that, in the class of catacondensed hexagonal systems, the minimum PI index is reached for the linear hexagon chain, while the maximum PI index is obtained for those systems in which each hexagon, apart from the terminal ones, is either angularly connected to two other hexagons or connected to three other hexagons. In [20], the lower and upper bound on the PI index of bicyclic graphs is given and the extremal graphs which get the bound are also given. However, in the class of all graphs on n-vertices, it is still an open question which graph attains the maximum PI index, see [8, 18] for detail.

In this paper, using the technique from [20], we give the lower bound on the PI index of connected tricyclic graphs and characterize the extremal graphs. The main result of this paper is the following theorem.

Theorem 1. *Let G be a connected tricyclic graph with m edges, then*

$$PI(G) \geq \begin{cases} m^2 - 4m, & \text{if } m = 4k \text{ for some } k, \\ m^2 - 4m + 4, & \text{if } m = 4k + 2 \text{ for some } k, \\ m^2 - 4m + 3, & \text{otherwise.} \end{cases}$$

When $m = 4k$, the graph in Figure 1 (a) with $p = q = r = s = k$ can get the minimum. When $m = 4k+1$, the graph in Figure 1 (a) with $p = q = r = s = k$ and with one pendant edge connecting to it can get the minimum. When $m = 4k + 2$, the graph in Figure 1 (a) with $p = q = r = k, s = k + 2$, or the graph (c) with $p = q = r = s = k, x = y = 1$ can get the minimum. When $m = 4k + 3$, the graph in Figure 1 (b) with $p = q = k, r = s = k + 1, x = 1$ can get the minimum.

Note that the contribution of each edge $e = (u, v)$ to $PI(G)$ is the number of edges which are not equidistant from its endpoints u and v. For the edges $e = (u, v)$ and e', define

$$\delta_{e=(u,v)}^{e'} = \begin{cases} 1, & d(u, e') = d(v, e') \\ 0, & d(u, e') \neq d(v, e') \end{cases} \tag{1}$$

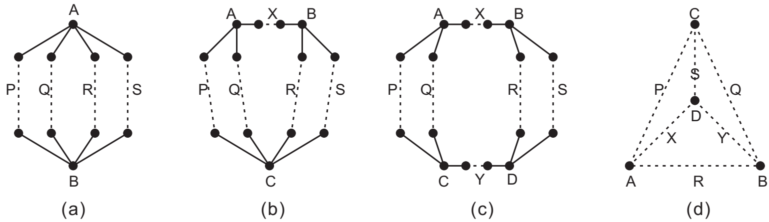

Figure 1. Braces of the graph in $\mathcal{T}_m^3$. The length of paths P, Q, R, S, X, Y is denoted by p, q, r, s, x, y respectively. In (a), all four paths P, Q, R, S are connecting vertices A and B. Similarly, all the paths are connecting two of the vertices among {A,B,C,D} in other three figures.

where $d(u, e')$ is the distance from vertex u to edge e'. Then $\sum_{e' \in E} \delta_e^{e'}$ is the number of edges that are equidistant to u and v. Define

$$S^*(G) = \sum_{e \in E} \sum_{e' \in E} \delta_e^{e'}. \tag{2}$$

$$PI(G) = \sum_{e \in E} [m - \sum_{e' \in E} \delta_e^{e'}] = m^2 - \sum_{e \in E} \sum_{e' \in E} \delta_e^{e'} = m^2 - S^*(G). \tag{3}$$

Note that $\delta_e^e = 1$ for every edge $e \in E$, $S^* = \sum_{e \in E} \delta_e^e + \sum_{e \in E} \sum_{e' \neq e} \delta_e^{e'} = m + \sum_{e \in E} \sum_{e' \neq e} \delta_e^{e'}$. In the following, compute $S^* - m$ via $S^* - m = \sum_{e \in E} \sum_{e' \neq e} \delta_e^{e'}$

If $e \in E$ is a cut edge, $\delta_e^{e'} = 0$ for any edge $e' \neq e$. So if $\delta_e^{e'} = 1 (e' \neq e)$, e should be in some cycle. If G is a even cycle with m edges, $\sum_{e \in E} \sum_{e' \in E \ e' \neq e} \delta_e^{e'} = m$.

Let $G = B_{p,q,r}$ be a bicyclic graph obtained from $P_{p+1} \cup P_{q+1} \cup P_{r+1}$ by identifying left endvertices as a new vertex, and identifying right endvertices as a new vertex. Suppose $P = P_{p+1}, Q = P_{q+1}, R = P_{r+1}$ and $p \leq q \leq r$ without loss of generality. In the following two cases, we will compute $S^* - m$ and the method will be used in the proof of the main theorem. First let p, q, r have the same parity, then the three even cycles PQ, PR, QR count $p + q, p + r, 2p$ respectively, so

$$S^*(G) - m = (p + q) + (p + r) + 2p \ .$$

Second let p has different parity with q, r, then the even cycle QR and the two odd cycles PQ, PR count $2(p + 1), 2\lfloor \frac{r-p}{2} \rfloor, 2\lfloor \frac{q-p}{2} \rfloor$ respectively, so

$$S^*(G) - m \leq 2(p + 1) + 2 \left\lfloor \frac{r - p}{2} \right\rfloor + 2 \left\lfloor \frac{q - p}{2} \right\rfloor \ .$$

Denote the set of tricyclic graphs with m edges by $\mathcal{T}_m$. For a graph $G \in \mathcal{T}_m$, if any two cycles do not have edges in common, then put G in subset $\mathcal{T}_m^1$; if G contains a bicyclic graph $B_{p,q,r}$ and an isolated cycle (cycle do not have common edge with the bicyclic graph), then put G in subset $\mathcal{T}_m^2$; If any cycle has common edges with at least one other cycle, then put G in subset $\mathcal{T}_m^3$. Note that any graph in $\mathcal{T}_m^3$ contains a subgraph of one of the four form in Figure 1, call them *brace*. It is easy to see that $\mathcal{T}_m = \mathcal{T}_m^1 \cup \mathcal{T}_m^2 \cup \mathcal{T}_m^3$.

Let P be a path and C be a cycle, denote the length of path P and cycle C by $L(P)$ and $L(C)$ respectively. Denote the edge set of path P and cycle C by $E(P)$ and $E(C)$ respectively. If $L(P) = 1$, denote the only edge of P by $e(P)$. In the following two sections, we give the proof of Theorem 1 by computing the upper bound of S^* for G in $\mathcal{T}_m^1, \mathcal{T}_m^2$ or $\mathcal{T}_m^3$.

2 The graphs in $\mathcal{T}_m^1$ or in $\mathcal{T}_m^2$

If $G \in \mathcal{T}_m^1$, denote the length of three cycles C_1, C_2, C_3 by x, y, z respectively.

1. All three cycles are even.

$S^* = m + x + y + z$. Because $x + y + z \leq m$ and $x, y, z \geq 4$, $m + 12 \leq S^* \leq 2m$.

2. Two cycles are even. Assume C_1, C_2 are even.

$S^* = m + x + y + (m - z) = 2m + x + y - z$. Because $8 \leq x + y \leq m - 3$ and $3 \leq z \leq m - 8$, $m + 16 \leq S^* \leq 3m - 6$

3. One cycle is even. Assume C_1 is even.

$S^* = m + x + (m - y) + (m - z) = 3m + x - y - z$. Because $4 \leq x \leq m - 6$, $y, z \geq 3$ and $y + z \leq m - 4$, $2m + 8 \leq S^* \leq 4m - 12$.

4. Every cycle is odd.

$S^* = m + (m - x) + (m - y) + (m - z)$. Because $x + y + z \leq m$ and $x, y, z \geq 3$, $3m \leq S^* \leq 4m - 9$

If $G \in \mathcal{T}_m^2$. Suppose the bicyclic graph in G is $B_{p,q,r}$, and the cycle that do not have common edges with $B_{p,q,r}$ is denoted by C. Let $p + q + r = m_1$, $L(C) = x$.

1. p, q, r are of the same parity and x is even. Note that $\sum_{e,e' \in E(B_{p,q,r})\ e \neq e'} \delta_e^{e'} \leq 2m_1$ and $\sum_{e \in E(B_{p,q,r})\ e' \in E(G) \setminus E(B_{p,q,r})} \delta_e^{e'} = 0$.

$S^* \leq m + 2m_1 + x$. Because $6 \leq m_1 \leq m - 4$, $4 \leq x \leq m - 6$ and $m_1 + x \leq m$, $S^* \leq 3m - 4$.

2. p, q, r are of the same parity and x is odd.

$S^* \leq m + 2m_1 + (m - x)$. Because $6 \leq m_1 \leq m - 3$, $3 \leq x \leq m - 6$ and $m_1 + x \leq m$, $S^* \leq 4m - 9$.

3. Not all of p, q, r are of the same parity and x is even. Note that $\sum_{e,e' \in E(B_{p,q,r})\ e \neq e'} \delta_e^{e'} \leq m_1 - 1$ and $\sum_{e \in E(B_{p,q,r})\ e' \in E(G) \setminus E(B_{p,q,r})} \delta_e^{e'} \leq 2(m - m_1)$.

$S^* \le m + (m_1 - 1) + 2(m - m_1) + x$. Because $5 \le m_1 \le m-4$, $4 \le x \le m-5$ and $m_1 + x \le m$, $S^* \le 4m - 11$.

4. Not all of p, q, r are of the same parity and x is odd.

$S^* \le m + (m_1 - 1) + 2(m - m_1) + (m - x)$. Because $5 \le m_1 \le m-3$, $3 \le x \le m-5$ and $m_1 + x \le m$, $S^* \le 4m - 9$.

3 The graphs in $\mathcal{T}_m^3$

For a graph $G \in \mathcal{T}_m^3$, the edges of G not in its brace are cut edges. Denote the brace of G by B and the number of cut edges of G by t. It is easy to see that

$$\sum_{e\in E(B)} \sum_{e\in E(G)\setminus E(B)} \delta_e^{e'} \le 3t \ .$$

In the following, assume graph G is one of the four braces in Figure 1. For an even cycle C in G, we said "compute via cycle C" means compute $\sum_{e\in E(C)\ e'\in E(C)\ e\neq e'} \delta_e^{e'}$. For an odd cycle C in G, we said "compute via cycle C" means compute $\sum_{e\in E(C)\ e'\in E(G)\ e\neq e'} \delta_e^{e'}$. Note that when C is an odd cycle, $\sum_{e\in E(C)\ e'\in E(C)\ e\neq e'} \delta_e^{e'} = 0$.

3.1 G is of the form in Figure 1(a)

Denote the length of path P, Q, R, S by p, q, r, s respectively. Without loss of generality, assume $p \le q \le r \le s$.

case 1. p, q, r, s have the same parity. Compute via even cycles PQ, PR, PS, QR, QS, RS subsequently.

$$\begin{aligned} S^* - m &= (p+q) + (p+r) + (p+s) + 2p + 2p + 2p \\ &= 3p + (q+2p) + (r+2p) + (s+2p) \le 3m \end{aligned}$$

When $p = q = r = s = k$ and $m = 4k$, $S^* = 4m$. When $p = q = r = k, s = k+2$ and $m = 4k+2$, $S^* = 4m - 4$.

case 2. One of p, q, r, s has different parity with another three.

2.1. p has different parity with q, r, s. Compute via even cycles QR, QS, RS and odd cycles PQ, PR, PS subsequently. Note that every even cycle count $2(p+1)$ and the odd cycles PQ, PR, PS count $2\lfloor\frac{r-p}{2}\rfloor + 2\lfloor\frac{s-p}{2}\rfloor, 2\lfloor\frac{s-p}{2}\rfloor + 2\lfloor\frac{q-p}{2}\rfloor, 2\lfloor\frac{r-p}{2}\rfloor + 2\lfloor\frac{q-p}{2}\rfloor$ respectively.

$$\begin{aligned} S^* - m &= 6(p+1) + 2\left(2\left\lfloor\frac{r-p}{2}\right\rfloor + 2\left\lfloor\frac{s-p}{2}\right\rfloor + 2\left\lfloor\frac{q-p}{2}\right\rfloor\right) \\ &= 6(p+1) + 2[(q-p-1) + (r-p-1) + (s-p-1)] \\ &= 2q + 2r + 2s < 3m - 4 \end{aligned}$$

2.2. q has different parity with p, r, s. Compute via even cycles PR, PS, RS and odd cycles PQ, QR, QS subsequently.

$$S^* - m = (p+r) + (p+s) + 2p + \left(2\left\lfloor\frac{r-p}{2}\right\rfloor + 2\left\lfloor\frac{s-p}{2}\right\rfloor\right) + 0 + 0 = 2p + 2r + 2s < 3m - 4$$

2.3. r has different parity with p, q, s. Compute via even cycles PQ, PS, QS and odd cycles PR, QR, RS subsequently.

$$S^* - m = (p+q) + (p+s) + 2p + \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{s-p}{2}\right\rfloor\right) + 0 + 0 = 2p + 2q + 2s < 3m - 4$$

2.4. s has different parity with p, q, r. Compute via even cycles PQ, PR, QR and odd cycles PS, QS, RS subsequently.

$$S^* - m = (p+q) + (p+r) + 2p + \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{r-p}{2}\right\rfloor\right) + 0 + 0 = 2p + 2q + 2r < 3m - 4$$

case 3. Two of p, q, r, s has different parity with another two.

3.1. p, q has different parity with r, s. Compute via even cycles PQ, RS and odd cycles PR, PS, QR, QS subsequently.

$$\begin{aligned} S^* - m &= (p+q) + 2(p+1) + \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{s-p}{2}\right\rfloor\right) + \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{r-p}{2}\right\rfloor\right) \\ &+ 0 + 0 = -p + 3q + r + s < 3m - 4 \end{aligned}$$

3.2. p, r has different parity with q, s. Compute via even cycles PR, QS and odd cycles PQ, PS, QR, RS subsequently.

$$\begin{aligned} S^* - m &= (p+r) + 2(p+1) + \left(2\left\lfloor\frac{r-p}{2}\right\rfloor + 2\left\lfloor\frac{s-p}{2}\right\rfloor\right) + \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{r-p}{2}\right\rfloor\right) \\ &+ 0 + 0 = -p + q + 3r + s < 3m - 4 \end{aligned}$$

3.3. p, s has different parity with q, r. Compute via even cycles PS, QR and odd cycles PQ, PR, QS, RS subsequently.

$$\begin{aligned} S^* - m &= (p+s) + 2(p+1) + \left(2\left\lfloor\frac{r-p}{2}\right\rfloor + 2\left\lfloor\frac{s-p}{2}\right\rfloor\right) + \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{s-p}{2}\right\rfloor\right) \\ &+ 0 + 0 = -p + q + r + 3s < 3m - 4 \end{aligned}$$

3.2 G is of the form in Figure 1(b)

Denote the length of path P, Q, R, S, X by p, q, r, s, x respectively. Without loss of generality, assume $p \leq q, r \leq s, p \leq r$.

case 1. $p, q, r+x, s+x$ have the same parity. Compute via even cycles PQ, PRX, PSX, QRX, RS, QSX subsequently.

$$\begin{aligned} S^* - m &\leq (p+q) + (p+r+x) + \begin{cases} p+x+s & p+x<r \\ 2r & p+x \geq r \end{cases} \\ &+ 2p + \begin{cases} 2(p+x) & p+x<r \\ r+s & p+x \geq r \end{cases} + 2p \\ &= \begin{cases} 9p+q+r+s+4x & p+x<r \\ 6p+q+4r+s+x & p+x \geq r \end{cases} \leq 3m-3 \end{aligned}$$

When $p = q = k, r = s = k+1, x = 1$ and $m = 4k+3$, $S^* = 4m-3$.

case 2. One of $p, q, r+x, s+x$ has different parity with another three.

2.1. p has different parity with $q, r+x, s+x$. Compute via even cycles QRX, RS, QSX and odd cycles PQ, PRX, PSX subsequently.

When $p+x<r$,

$$\begin{aligned} S^* - m &\leq 2(p+1) + 2(p+x+1) + 2\min\{p+1, r\} \\ &+ \left(2\left\lfloor\frac{r+x-p}{2}\right\rfloor + 2\left\lfloor\frac{s+x-p}{2}\right\rfloor\right) + \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{s-p-x}{2}\right\rfloor\right) \\ &+ \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{r-p-x}{2}\right\rfloor\right) = 2q+2r+2s+2x < 3m-4\ . \end{aligned}$$

When $r \leq p+x$,

$$\begin{aligned} S^* - m &\leq 2(p+1) + (r+s) + 2\min\{p+1, r\} \\ &+ \left(2\left\lfloor\frac{r+x-p}{2}\right\rfloor + 2\left\lfloor\frac{s+x-p}{2}\right\rfloor\right) + \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{s-r}{2}\right\rfloor\right) \\ &+ 2\left\lfloor\frac{q-p}{2}\right\rfloor = 2q+r+3s+2x < 3m-4\ . \end{aligned}$$

2.2. q has different parity with $p, r+x, s+x$. Compute via even cycles PRX, PSX, RS and odd cycles PQ, QRX, QSX subsequently.

When $p+x<r$,

$$\begin{aligned}S^*-m &\le (p+r+x)+(p+s+x)+2(p+x)\\ &+ \left(2\left\lfloor\frac{r+x-p}{2}\right\rfloor+2\left\lfloor\frac{s+x-p}{2}\right\rfloor-x\right)+\begin{cases}0 & q+x<r\\ 2\left\lfloor\frac{s-r}{2}\right\rfloor & q+x>r\end{cases}+0\\ &= \begin{cases}2p+2r+2s+5x & q+x<r\\ 2p+r+3s+5x & q+x>r\end{cases}<3m-4\ .\end{aligned}$$

When $p+x\ge r$,

$$\begin{aligned}S^*-m &\le (p+r+x)+2r+(r+s)\\ &+ \left(2\left\lfloor\frac{r+x-p}{2}\right\rfloor+2\left\lfloor\frac{s+x-p}{2}\right\rfloor-\min\left\{x,\lfloor\frac{r+x-p}{2}\rfloor\right\}\right)\\ &+ 2\left\lfloor\frac{s-r}{2}\right\rfloor+0=\begin{cases}-p+4r+3s+2x & x<\lfloor\frac{r+x-p}{2}\rfloor\\ -\frac{1}{2}p+\frac{7}{2}r+3s+\frac{5}{2}x & x\ge\lfloor\frac{r+x-p}{2}\rfloor\end{cases}<3m-4\ .\end{aligned}$$

2.3. $r+x$ has different parity with $p,q,s+x$. Compute via even cycles PQ,PSX,QSX and odd cycles PRX,QRX,RS subsequently.

When $p+x>r$,

$$\begin{aligned}S^*-m &\le (p+q)+2(r+1)+2\min\{p,r+1\}\\ &+ \left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-r}{2}\right\rfloor\right)+2\left\lfloor\frac{s-r}{2}\right\rfloor+\left(2\left\lfloor\frac{p+x-r}{2}\right\rfloor+2\left\lfloor\frac{q+x-r}{2}\right\rfloor\right)\\ &= 3p+3q-2r+2s+2x-2<3m-4\ .\end{aligned}$$

When $p+x<r$,

$$\begin{aligned}S^*-m &\le (p+q)+(p+x+s)+2\min\{p,r+1\}\\ &+ \left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-p-x}{2}\right\rfloor\right)+0+0\\ &= 2p+2q+2s<3m-4\ .\end{aligned}$$

2.4. $s+x$ has different parity with $p,q,r+x$. Compute via even cycles PQ,PRX,QRX and odd cycles PSX,RS,QSX subsequently.

When $p+x\ge r$,

$$\begin{aligned}S^*-m &\le (p+q)+(p+r+x)+2p+2\left\lfloor\frac{q-p}{2}\right\rfloor+\left(2\left\lfloor\frac{p+x-r}{2}\right\rfloor+2\left\lfloor\frac{q+x-r}{2}\right\rfloor\right)\\ &+ 0=4p+3q-r+3x<3m-4\ .\end{aligned}$$

When $p+x<r$,

$$\begin{aligned} S^*-m &\le (p+q)+(p+r+x)+2p \\ &+ \left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{r-p-x}{2}\right\rfloor\right)+0+0=2p+2q+2r<3m-4\ . \end{aligned}$$

case 3. Two of $p,q,r+x,s+x$ has different parity with another two.

3.1. p,q has different parity with $r+x,s+x$. Compute via even cycles PQ,RS and odd cycles PRX,PSX,QRX,QSX subsequently.

When $p+x>r$,

$$\begin{aligned} S^*-m &\le (p+q)+(r+s)+\left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-r}{2}\right\rfloor\right) \\ &+ 2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-r}{2}\right\rfloor+0=-p+3q-r+3s<3m-4\ . \end{aligned}$$

When $p+x<r$,

$$\begin{aligned} S^*-m &\le (p+q)+2(p+x+1)+\left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-p-x}{2}\right\rfloor\right) \\ &+ \left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{r-p-x}{2}\right\rfloor\right)+0+0\ =-p+3q+r+s<3m-4\ . \end{aligned}$$

3.2. $p,r+x$ has different parity with $q,s+x$. Compute via even cycles PRX,QSX and odd cycles PQ,PSX,QRX,RS subsequently. In the computation of equidistant edges via some cycles, some minus happen because some repeat count happens.

When $p+x\ge r$,

$$\begin{aligned} S^*-m &\le (p+r+x)+2(p+1)+\left(2\left\lfloor\frac{r+x-p}{2}\right\rfloor+2\left\lfloor\frac{s+x-p}{2}\right\rfloor-\left\lfloor\frac{r+x-p}{2}\right\rfloor\right. \\ &- \left.\max\left\{0,\left\lfloor\frac{s+x-p}{2}\right\rfloor-s\right\}\right)+2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-r}{2}\right\rfloor+\left(2\left\lfloor\frac{p+x-r}{2}\right\rfloor\right. \\ &+ \left.2\left\lfloor\frac{q+x-r}{2}\right\rfloor-\left\lfloor\frac{p+x-r}{2}\right\rfloor-\max\left\{0,\left\lfloor\frac{q+x-r}{2}\right\rfloor-q\right\}\right) \\ &= p+2q-r+2s+4x-2-\max\left\{0,\left\lfloor\frac{s+x-p}{2}\right\rfloor-s\right\} \\ &- \max\left\{0,\left\lfloor\frac{q+x-r}{2}\right\rfloor-q\right\}<3m-4\ . \end{aligned}$$

When $p+x<r$,

$$\begin{aligned} S^*-m &\le (p+r+x)+2(p+1)+\left(2\left\lfloor\frac{r+x-p}{2}\right\rfloor+2\left\lfloor\frac{s+x-p}{2}\right\rfloor-x\right) \\ &+ \left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{r-p-x}{2}\right\rfloor\right)+0+0=-p+q+3r+s+x<3m-4\ . \end{aligned}$$

3.3. $p, s+x$ has different parity with $q, r+x$. Compute via even cycles PSX, QRX and odd cycles PQ, PRX, RS, QSX subsequently.

When $p+x>r$,

$$\begin{aligned} S^*-m &\leq 2(r+1)+2(p+1)+\left(2\left\lfloor\frac{r+x-p}{2}\right\rfloor+2\left\lfloor\frac{s+x-p}{2}\right\rfloor-\left\lfloor\frac{r+x-p}{2}\right\rfloor\right. \\ &- \left.\max\left\{0,\left\lfloor\frac{s+x-p}{2}\right\rfloor-s\right\}\right)+\left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-r}{2}\right\rfloor\right) \\ &+ \left(2\left\lfloor\frac{p+x-r}{2}\right\rfloor+2\left\lfloor\frac{q+x-r}{2}\right\rfloor-\left\lfloor\frac{p+x-r}{2}\right\rfloor\right. \\ &- \left.\max\left\{0,\left\lfloor\frac{q+x-r}{2}\right\rfloor-q\right\}\right)+0 \leq 2p+2s+3x-3<3m-4\ . \end{aligned}$$

When $p+x<r$,

$$\begin{aligned} S^*-m &\leq (p+s+x)+2(p+1)+\left(2\left\lfloor\frac{r+x-p}{2}\right\rfloor+2\left\lfloor\frac{s+x-p}{2}\right\rfloor-x\right) \\ &+ \left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-p-x}{2}\right\rfloor\right)+0+0=-p+q+r+3s+x<3m-4\ . \end{aligned}$$

3.3 G is of the form in Figure 1(c)

Denote the length of path P, Q, R, S, X, Y by p, q, r, s, x, y respectively. Without loss of generality, assume $p \leq q, r \leq s, p \leq r, x \leq y$.

case 1. $p, q, r+x+y, s+x+y$ have the same parity. Compute via even cycles $PQ, PXRY, PXSY, QXRY, RS, QXSY$ subsequently.

When $p+x+y<r$,

$$\begin{aligned} S^*-m &= (p+q)+(p+r+x+y)+(p+s+x+y)+2p+2(p+x+y)+2p \\ &= 9p+q+r+s+4x+4y<3p+3q+3r+3s<3m-4\ . \end{aligned}$$

When $p+x+y \geq r$,

$$\begin{aligned} S^*-m &= (p+q)+(p+r+x+y)+2r+2p+(r+s)+2p \\ &= 6p+q+4r+s+x+y \leq 3p+3q+3r+3s+x+y \leq 3m-4\ . \end{aligned}$$

When $p=q=r=s=k$, $x=y=1$ and $m=4k+2$, $S^*=4m-4$.

case 2. One of $p, q, r+x+y, s+x+y$ has different parity with another three.

2.1. p has different parity with $q, r+x+y, s+x+y$. Compute via even cycles $QXRY, RS, QXSY$ and odd cycles $PQ, PXRY, PXSY$ subsequently.

When $p+x+y<r$,

$$\begin{aligned} S^*-m &\leq 2(p+1)+2(p+x+y+1)+2(p+1) \\ &+ \left(2\left\lfloor\frac{r+x+y-p}{2}\right\rfloor+2\left\lfloor\frac{s+x+y-p}{2}\right\rfloor\right) \\ &+ \left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-p-x-y}{2}\right\rfloor\right)+\left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{r-p-x-y}{2}\right\rfloor\right) \\ &= 2q+2r+2s+2x+2y<3m-4 \ . \end{aligned}$$

When $p+x+y>r$,

$$\begin{aligned} S^*-m &\leq 2(p+1)+(r+s)+2(p+1) \\ &+ \left(2\left\lfloor\frac{r+x+y-p}{2}\right\rfloor+2\left\lfloor\frac{s+x+y-p}{2}\right\rfloor\right)+\left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-r}{2}\right\rfloor\right) \\ &+ 2\left\lfloor\frac{q-p}{2}\right\rfloor=2q+r+3s+2x+2y<3m-4 \ . \end{aligned}$$

2.2. q has different parity with $p, r+x+y, s+x+y$. Compute via even cycles $PXRY, PXSY, RS$ and odd cycles $PQ, QXRY, QXSY$ subsequently.

When $p+x+y<r$,

$$\begin{aligned} S^*-m &\leq (p+r+x+y)+(p+s+x+y)+2(p+x+y) \\ &+ \left(2\left\lfloor\frac{r+x+y-p}{2}\right\rfloor+2\left\lfloor\frac{s+x+y-p}{2}\right\rfloor-(x+y)\right) \\ &+ \begin{cases} 0 & q<r+x+y \\ 2\left\lfloor\frac{s-r}{2}\right\rfloor & q>r+x+y \end{cases} +0 \\ &= \begin{cases} 2p+2r+2s+5x+5y\leq 3r+3s+3x+3y<3m-4 & q<r+x+y \\ 2p+r+3s+5x+5y\leq 3r+3s+3x+3y<3m-4 & q>r+x+y \end{cases} . \end{aligned}$$

When $p+x+y\geq r$,

$$\begin{aligned} S^*-m &\leq (p+r+x+y)+2r+(r+s) \\ &+ \left(2\left\lfloor\frac{r+x+y-p}{2}\right\rfloor+2\left\lfloor\frac{s+x+y-p}{2}\right\rfloor-\min\left\{x,\left\lfloor\frac{r+x+y-p}{2}\right\rfloor\right\}\right. \end{aligned}$$

$$- \quad \min\left\{y, \left\lfloor\frac{r+x+y-p}{2}\right\rfloor\right\}\Bigg) + 2\left\lfloor\frac{s-r}{2}\right\rfloor + 0$$

$$= \begin{cases} -p+4r+3s+2x+2y < 3m-4 & \lfloor\frac{r+x+y-p}{2}\rfloor \geq y \\ -\frac{1}{2}p+\frac{7}{2}r+3s+\frac{3}{2}x+\frac{5}{2}y < 3m-4 & x < \lfloor\frac{r+x+y-p}{2}\rfloor < y \\ 3r+3s+2x+2y < 3m-4 & \lfloor\frac{r+x+y-p}{2}\rfloor \leq x \end{cases} .$$

2.3. $r+x+y$ has different parity with $p, q, s+x+y$. Compute via even cycles $PQ, PXSY, QXSY$ and odd cycles $PXRY, QXRY, RS$ subsequently.

When $p+x+y > r$,

$$\begin{aligned} S^* - m &\leq (p+q) + 2(r+1) + 2p + \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{s-r}{2}\right\rfloor\right) \\ &+ 2\left\lfloor\frac{s-r}{2}\right\rfloor + \left(2\left\lfloor\frac{p+x+y-r}{2}\right\rfloor + 2\left\lfloor\frac{q+x+y-r}{2}\right\rfloor\right) \\ &= 3p+3q-2r+2s+2x+2y-2 < 3m-4 \ . \end{aligned}$$

When $p+x+y < r$,

$$\begin{aligned} S^* - m &\leq (p+q) + (p+s+x+y) + 2p + \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{s-p-x-y}{2}\right\rfloor\right) \\ &+ 0 + 0 = 2p+2q+2s < 3m-4 \ . \end{aligned}$$

2.4. $s+x+y$ has different parity with $p, q, r+x+y$. Compute via even cycles $PQ, PXRY, QXRY$ and odd cycles $PXSY, RS, QXSY$ subsequently.

When $p+x+y \geq r$,

$$\begin{aligned} S^* - m &\leq (p+q) + (p+r+x+y) + 2p + 2\left\lfloor\frac{q-p}{2}\right\rfloor \\ &+ \left(2\left\lfloor\frac{p+x+y-r}{2}\right\rfloor + 2\left\lfloor\frac{q+x+y-r}{2}\right\rfloor\right) + 0 \\ &= 4p+3q-r+3x+3y < 3m-4 \ . \end{aligned}$$

When $p+x+y < r$,

$$\begin{aligned} S^* - m &\leq (p+q) + (p+r+x+y) + 2p + \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{r-p-x-y}{2}\right\rfloor\right) \\ &+ 0 + 0 = 2p+2q+2r < 3m-4 \ . \end{aligned}$$

case 3. Two of $p, q, r+x+y, s+x+y$ has different parity with another two.

3.1. p, q has different parity with $r+x+y, s+x+y$. Compute via even cycles PQ, RS and odd cycles $PXRY, PXSY, QXRY, QXSY$ subsequently.

When $p+x+y>r$,

$$S^*-m \le (p+q)+(r+s)+\left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-r}{2}\right\rfloor\right)$$
$$+\ 2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-r}{2}\right\rfloor+0=-p+3q-r+3s<3m-4\ .$$

When $p+x+y<r$,

$$S^*-m \le (p+q)+2(p+x+y+1)+\left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{s-p-x-y}{2}\right\rfloor\right)$$
$$+\ \left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{r-p-x-y}{2}\right\rfloor\right)+0+0=-p+3q+r+s<3m-4\ .$$

3.2. $p, r+x+y$ has different parity with $q, s+x+y$. Compute via even cycles $PXRY, QXSY$ and odd cycles $PQ, PXSY, QXRY, RS$ subsequently.

When $p+x+y\ge r$,

$$S^*-m \le (p+r+x+y)+2(p+1)+\left[2\left\lfloor\frac{r+x+y-p}{2}\right\rfloor+2\left\lfloor\frac{s+x+y-p}{2}\right\rfloor\right.$$
$$-\ \left.\min\left\{\left\lfloor\frac{r+x+y-p}{2}\right\rfloor,x\right\}-\min\left\{\left\lfloor\frac{r+x+y-p}{2}\right\rfloor,y\right\}\right]+2\left\lfloor\frac{q-p}{2}\right\rfloor$$
$$+\ 2\left\lfloor\frac{s-r}{2}\right\rfloor+\left[2\left\lfloor\frac{p+x+y-r}{2}\right\rfloor+2\left\lfloor\frac{q+x+y-r}{2}\right\rfloor\right.$$
$$-\ \left.\min\left\{\left\lfloor\frac{p+x+y-r}{2}\right\rfloor,x\right\}-\min\left\{\left\lfloor\frac{p+x+y-r}{2}\right\rfloor,y\right\}\right]<3m-4\ .$$

When $p+x+y<r$,

$$S^*-m \le (p+r+x+y)+2(p+1)+\left(2\left\lfloor\frac{r+x+y-p}{2}\right\rfloor+2\left\lfloor\frac{s+x+y-p}{2}\right\rfloor\right)$$
$$+\ \left(2\left\lfloor\frac{q-p}{2}\right\rfloor+2\left\lfloor\frac{r-p-x-y}{2}\right\rfloor\right)+0+0=-p+q+3r+s+2x+2y$$
$$<\ 3m-4\ .$$

3.3. $p, s+x+y$ has different parity with $q, r+x+y$. Compute via even cycles $PXSY, QXRY$ and odd cycles $PQ, PXRY, RS, QXSY$ subsequently.

When $p+x+y>r$,

$$S^*-m \le 2(r+1)+2(p+1)+\left[2\left\lfloor\frac{r+x+y-p}{2}\right\rfloor+2\left\lfloor\frac{s+x+y-p}{2}\right\rfloor\right.$$
$$-\ \left.\min\left\{\left\lfloor\frac{r+x+y-p}{2}\right\rfloor,x\right\}-\min\left\{\left\lfloor\frac{r+x+y-p}{2}\right\rfloor,y\right\}\right]$$

$$+ \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{s-r}{2}\right\rfloor\right) + \left[2\left\lfloor\frac{p+x+y-r}{2}\right\rfloor + 2\left\lfloor\frac{q+x+y-r}{2}\right\rfloor\right.$$

$$\left. - \min\left\{\left\lfloor\frac{p+x+y-r}{2}\right\rfloor, x\right\} - \min\left\{\left\lfloor\frac{p+x+y-r}{2}\right\rfloor, y\right\}\right] + 0 < 3m-4\ .$$

When $p+x+y<r$,

$$\begin{aligned} S^*-m &\leq (p+s+x+y)+2(p+1) \\ &+ \left(2\left\lfloor\frac{r+x+y-p}{2}\right\rfloor + 2\left\lfloor\frac{s+x+y-p}{2}\right\rfloor\right) \\ &+ \left(2\left\lfloor\frac{q-p}{2}\right\rfloor + 2\left\lfloor\frac{s-p-x-y}{2}\right\rfloor\right) + 0 + 0 \\ &= -p+q+r+3s+2(x+y) < 3m-4\ . \end{aligned}$$

3.4 G is of the form in Figure 1(d)

In this section, when $\delta_e^{e'}=1$ via an even cycle, it is easy to see that $\delta_{e'}^{e}=1$. We said "e and e' count 1" respectively in this case. When $\delta_e^{e_1}=1$ via an odd cycle, it is easy to see that $\delta_{e_1}^{e}=0$. There may have some other edges e_i $(2\leq i\leq t)$ except e_1 such that $\delta_e^{e_i}=1$ and e_i is adjacent to e_{i+1} $(1\leq i\leq t-1)$. We said "e and e_i $(1\leq i\leq t)$ count $\frac{t}{t+1}$" respectively in this case. Note that every edge e count once via a cycle and three cycles will contain all six paths P,Q,R,S,X,Y, so e will count no more than 3 except $\delta_e^e=1$ and we know $S^*\leq 4m$. In the following, we will prove $S^*\leq 4m-4$.

Assume path R is the longest path among P,Q,R,S,X,Y and $L(R)=r$. There are four paths from A to B except R, which are XY,PQ,XSQ,PSY. Consider the closest one. By symmetry only two need to be considered.

Denote the length of the closest path from A to B except R by r_1. If $r-r_1\geq 2$, it is easy to see that $S^*\leq 4m-4$ in this case. Next assume $r-r_1=1$.

First assume the closest path from A to B except R is XY without loss of generality. If $r\geq 4$, the cycle RXY has at least 7 edges, and at least 4 edges in the cycle count no more than 2, so $S^*\leq 4m-4$. If the length of path R is 3, then the length of path X,Y is 1, the other three paths P,S,Q may have $1,2$ or 3 edges. It is easy to prove that $S^*\leq 4m-4$ in every case. The length of path R cannot be 2.

Now assume the the closest path from A to B except R is XSQ without loss of generality. If $r\geq 5$, the cycle $RXSQ$ has at least 9 edges, and at least 5 edges in the cycle count at most 2, so $S^*<4m-4$. If the length of path R is 4, then the length of path X,S,Q is 1 respectively, the other two paths P,Y may have 3 or 4 edges. It is easy to prove that

$S^* \leq 4m - 4$ in every case. The length of path R cannot be 3.

In the following, only consider the graph with the property that the closest path from A to B except R is greater than or equal to the length of path R ($r \leq r_1$).

case 1. Assume the closest path from A to B except R is XY and the cycle RXY is odd.

Among all the edges in cycle RXY, only three edges, which are the edges of equidistance to A, B, D respectively, may count more than 2. All other edges in cycle RXY count at most 2. When $L(R) \geq 3$, the length of cycle RXY is at least 7. In this case, $S^* \leq 4m - 4$ obviously. When $L(R) = 2$, suppose $L(X) = 1$ and $L(Y) = 2$ without loss of generality, the length of P, Q, S may be 1 or 2 and $L(PQ) \geq 3$, it is easy to see that in all these cases $S^* \leq 4m - 4$.

case 2. Assume the closest path from A to B except R is XSQ and the cycle $RXSQ$ is odd.

If $L(PQ) \leq L(XSQ)$ or $L(XY) \leq L(XSQ)$, above discussion proves $S^* \leq 4m-4$. So assume $L(PQ) > L(XSQ)$ and $L(XY) > L(XSQ)$. In cycle $RXSQ$, four edges, which are the edges of equidistance to A, B, C, D respectively, may count more than two. All other edges count at most 2. When the length of R is at least 4, the length of cycle $RXSQ$ is at least 9, $S^* < 4m - 4$ obviously. The length of path R cannot be 2 or 3 because $L(PQ) > L(XSQ)$ and $L(XY) > L(XSQ)$, so $S^* \leq 4m - 4$ in this case.

case 3. Assume the closest path from A to B except R is XY and the cycle RXY is even.

3.1. Assume the cycle RPQ is odd.

In this case, one of the two cycles PXS and QYS is of even length and the other one is of odd length. Suppose the cycle PXS is of odd length, the cycle $RXSQ$ is even and the cycle $RPSY$ is odd now. Because every cycle contained P is odd, every edge in P count at most 1. When $L(P) \geq 2$, $S^* \leq 4m - 4$. When $L(P) = 1$, it is easy to see that every edge in R counts at most 2, so $S^* \leq 4m - 4$.

3.2 Assume the cycle RPQ is even.

In this case, both cycles PXS and QYS have the same parity.

3.2.1 Both cycles PXS and QYS are odd.

Because both $L(PXS)$ and $L(QSY)$ are odd, every edge in X, Y or S count at most 2. When $L(X) + L(Y) + L(S) \geq 4$, $S^* \leq 4m - 4$. When $L(X) + L(Y) + L(S) = 3$, this happens when $L(R) = 2, L(P) = L(Q) = L(X) = L(Y) = L(S) = 1$, it is easy to see that $S^* \leq 4m - 4$ in this case.

3.2.2 Both cycles PXS and QYS are even.

All cycles are even now. Suppose the edge adjacent A in path R is e_1 and the edge adjacent B in path R is e_2. The edge e_1 may be count via three cycles $RXY, RPQ, RXSQ$ and it cannot be count via cycle $RYSP$. The edge e_1 count once via cycle RXY. Suppose $L(P) \leq L(XS)$ without loss of generality, the edge e_1 count once via cycle RPQ. It cannot be count via cycle $RXSQ$. Suppose the equidistant edge of e_1 via cycle $RXSQ$ is $e^{'}$. The distance between vertex A and edge $e^{'}$ via P is less than that via XSQ. So edge e_1 can only be count 2. Similar discussion can prove that the edge e_2 also counts 2. If there is a path among $\{P, Q, S, X, Y\}$ whose length equals to $L(P)$, $S^* \leq 4m - 4$ because there are at least four edges count 2. Next suppose $max\{L(P), L(Q), L(X), L(Y), L(S)\} < L(R)$.

Divide the edge set of path R into two sets $E_A(R)$ and $E_B(R)$. $E_A(R)$ denote the edges in path R such that it reach D via RX closer than via RY. $E_B(R)$ denote the edges in path R such that it reach D via RY closer than via RX. The edges in $E_A(R)$ may count via cycles $RXY, RPQ, RXSQ$ and the edges in $E_B(R)$ may count via cycles $RXY, RPQ, RYSP$. If there is an edge in $E_B(R)$ ($E_A(R)$) which count 3, any edge in $E_A(R)$ ($E_B(R)$) count 2. Suppose if there are some edges in path R count 3, they are in $E_B(R)$. Note that $|E_A(R)| \geq 1$.

Suppose $L(X) \geq L(Y)$, for $L(X) < L(R) = r, L(Y) < L(R)$, so $L(X) - L(Y) \leq r - 2$. $L(X) - L(Y)$ has the same parity with r because RXY is even. If $L(X) - L(Y) \leq r - 6$ ($r \geq 6$), $|E_A(R)| \geq 3$, so $S^* \leq 4m - 4$.

If $L(X) - L(Y) = r - 2$, $L(X)$ should be $r - 1$ and $L(Y)$ should be 1. In this case $|E_A(R)| = 1$ and $|E_B(R)| = r - 1$. If there is only one edge in $E_B(R)$ counts 2, this happens when $L(Q) = r - 1, L(P) = 1, L(S) = r - 2$. The edges $e(P)$ and $e(Y)$ count 2. So $S^* \leq 4m - 4$.

If there are two edges in $E_B(R)$ count 2, $L(Q), L(P), L(S)$ may be $r - 2, 2, r - 3$ or $r - 1, 3, r - 2$. When $L(Q) = r - 2, L(P) = 2, L(S) = r - 3$, the two edges in $E(P)$ count 2, so $S^* < 4m - 4$. When $L(Q) = r - 1, L(P) = 3, L(S) = r - 2$, the edge $e(Y)$ counts 2, so $S^* \leq 4m - 4$.

If there are three edges in $E_B(R)$ count 2, $S^* \leq 4m - 4$.

If $L(X) - L(Y) = r - 4$, $L(X), L(Y)$ may be $r - 2, 2$ or $r - 1, 3$. In this case $|E_A(R)| = 2$ and $|E_B(R)| = r - 2$. When $L(X) = r - 2, L(Y) = 2$, if there is only one edge in $E_B(R)$ counts 2, this happens when $L(Q) = r - 1, L(P) = 1, L(S) = r - 3$. $e(P)$ counts 2, so $S^* \leq 4m - 4$. If there are at least two edges in $E_B(R)$ count 2, $S^* \leq 4m - 4$.

When $L(X) = r - 1, L(Y) = 3$, there are at least two edges in $E_B(R)$ count 2 because $L(XY) \leq L(PQ)$, so $S^* \leq 4m - 4$.

case 4. Assume the closest path from A to B except R is XSQ and the cycle $RXSQ$ is even.

In this case, from the above discussion, assume $L(S)+L(Q)<L(Y), L(X)+L(S)<L(P)$. If $L(X)=1$, $L(S)+L(Q)\geq r-1$, so $L(S)+L(Q)=r-1$, $L(Y)=r$. Because cycle RXY is odd, at least $L(RXY)-3$ edges in RXY count at most 2. $L(R)=r\geq 3$, $L(RXY)=2r+1\geq 7$, so $S^*\leq 4m-4$. Next assume $L(X)\geq 2, L(Q)\geq 2$.
If $L(X)=2$, $L(S)+L(Q)\geq r-2$. In this case, $L(S)+L(Q)=r-2$, $L(Y)=r-1$ or $L(Y)=r$,$r\geq 5$. When $L(Y)=r-1$, because RXY is odd, there are at least $r-1\geq 4$ edges in path R which count at most 2, so $S^*\leq 4m-4$. When $L(Y)=r$, the two edges in X and the two edges in R nearer to A count at most 2, so $S^*\leq 4m-4$.
Next assume $L(X)\geq 3, L(Q)\geq 3$, $r\geq 5$ now. When RXY or RPQ is odd, there are at least $r-1\geq 4$ edges in R count at most 2. Assume both RXY and RPQ are even. Because $L(S)+L(Q)<L(Y), L(X)+L(S)<L(P)$, the two edges in R nearer to A and the two edges in R nearer to B count at most 2, so $S^*\leq 4m-4$.

Remark: A similar and more precise discussion will prove that $S^*<4m-4$ in all the cases of this subsection.

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