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On Bounds for Harmonic Topological Index

Marjan Matejić[a], Igor Milovanović[a], Emina Milovanović[a]

[a]*Faculty of Electronics Engineering, University of Niš, A. Medvedeva 14, 18000 Niš, Serbia*

Abstract. Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be a simple graph with n vertices and m edges. Denote by $d_1 \geq d_2 \geq \cdots \geq d_n > 0$ and $d(e_1) \geq d(e_2) \geq \cdots \geq d(e_m)$, sequences of vertex and edge degrees, respectively. If i-th and j-th vertices of the graph G are adjacent, it is denoted as $i \sim j$. Graph invariant referred to as harmonic index is defined as $H(G) = \sum_{i \sim j} \frac{2}{d_i + d_j}$. Lower and upper bounds for invariant $H(G)$ are obtained.

1. Introduction

Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be a simple graph. Denote by $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, and $d(e_1) \geq d(e_2) \geq \cdots \geq d(e_m)$, sequences of vertex and edge degrees, respectively. In addition, we use the following notation: $\Delta = d_1$, $\delta = d_n$, $\Delta_{e_1} = d(e_1) + 2$, $\Delta_{e_2} = d(e_2) + 2$, $\delta_{e_1} = d(e_m) + 2$, $\delta_{e_2} = d(e_{m-1}) + 2$. If i-th and j-th vertices (e_i and e_j edges) of the graph G are adjacent, it is denoted as $i \sim j$ ($e_i \sim e_j$). As usual, $L(G)$ denotes a line graph of G.

Gutman and Trinajstić [9] introduced two vertex degree topological indices, named the first and the second Zagreb indices. These are defined as

$$M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2 \qquad \text{and} \qquad M_2 = M_2(G) = \sum_{i \sim j} d_i d_j .$$

The first Zagreb index can be also expressed as

$$M_1 = M_1(G) = \sum_{i \sim j} (d_i + d_j) \,. \tag{1}$$

Details on the mathematical theory of Zagreb indices can be found in [1, 4–8].

In [18] Zhou and Trinajstić defined general sum-connectivity index H_α, as

$$H_\alpha = H_\alpha(G) = \sum_{i \sim j} (d_i + d_j)^\alpha ,$$

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Email addresses: marjan.matejic@elfak.ni.ac.rs (Marjan Matejić), igor@elfak.ni.ac.rs (Igor Milovanović), ema@elfak.ni.ac.rs (Emina Milovanović)

where α is an arbitrary real number.

Here we are concerned with two special variants of H_α, the sum-connectivity index $X = H_{-1/2}$ [19], and harmonic topological index $H = 2H_{-1}$ [3], which are defined as

$$X = X(G) = \sum_{i\sim j} \frac{1}{\sqrt{d_i + d_j}} \quad \text{and} \quad H = H(G) = \sum_{i\sim j} \frac{2}{d_i + d_j}\,. \tag{2}$$

2. Preliminaries

In what follows, we outline a few inequalities for topological index H as well as some analytical inequalities that will be needed in the subsequent considerations.

Rodrigues and Sigarreta [14] have determined the following upper bound for index H in terms of invariant M_1 and graph parameters m, Δ and δ

$$H \le \frac{m^2}{2M_1}\left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2, \tag{3}$$

with equality if G is regular.

Ilić [11] and Xu [17] independently proved the following inequality involving the harmonic and the first Zagreb indices

$$H \ge \frac{2m^2}{M_1}\,, \tag{4}$$

with equality if and only if $d_i + d_j$ is constant for each pair of adjacent vertices i and j.

Having in mind (1) and (2) it can be easily observed that topological indices M_1, X and H can be computed according to

$$M_1 = \sum_{i=1}^{m}(d(e_i) + 2)\,, \qquad X = \sum_{i=1}^{m} \frac{1}{\sqrt{d(e_i) + 2}}\,, \quad \text{and} \quad H = \sum_{i=1}^{m} \frac{2}{d(e_i) + 2}\,. \tag{5}$$

Let $a = (a_i)$, $i = 1, 2, \ldots, m$, be a sequence of positive real numbers with the property $0 < r \le a_i \le R < +\infty$. Szökefalvi Nagy [16] (see also [15]) proved that

$$m\sum_{i=1}^{m} a_i^2 - \left(\sum_{i=1}^{m} a_i\right)^2 \ge \frac{m}{2}(R - r)^2\,. \tag{6}$$

Let d and s be non-negative real numbers so that $d > s \ge 0$. Then, equality in (6) is attained for $R = a_1 = d + s$, $d = a_2 = \cdots = a_{m-1}$ and $r = d - s = a_m$.

Denote with $p = (p_i)$ and $a = (a_i)$ sequences of real numbers with the properties

$$p_i \ge 0, \qquad \sum_{i=1}^{m} p_i = 1, \qquad 0 < r \le a_i \le R < +\infty\,, \quad i = 1, 2, \ldots, m\,.$$

In [10] Henrici proved that

$$\sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} \frac{p_i}{a_i} \le \frac{1}{4}\left(\sqrt{\frac{R}{r}} + \sqrt{\frac{r}{R}}\right)^2\,. \tag{7}$$

Similarly, in [12] Lupas proved that

$$\sum_{i=1}^{m} a_i \sum_{i=1}^{m} \frac{1}{a_i} \le \frac{\left(\left\lfloor \frac{m}{2}\right\rfloor R + \left\lfloor \frac{m+1}{2}\right\rfloor r\right)\left(\left\lfloor \frac{m+1}{2}\right\rfloor R + \left\lfloor \frac{m}{2}\right\rfloor r\right)}{Rr}\,. \tag{8}$$

We'll show that this inequality can also be represented in the following form

$$\sum_{i=1}^{m} a_i \sum_{i=1}^{m} \frac{1}{a_i} \le m^2 \left(1 + \alpha(m)\left(\sqrt{\frac{R}{r}} - \sqrt{\frac{r}{R}}\right)^2\right), \tag{9}$$

where

$$\alpha(m) = \frac{1}{4}\left(1 - \frac{(-1)^{m+1}+1}{2m^2}\right).$$

Suppose, first, that m is even. Then

$$\begin{aligned}\frac{\left(\left\lfloor\frac{m}{2}\right\rfloor R + \left\lfloor\frac{m+1}{2}\right\rfloor r\right)\left(\left\lfloor\frac{m+1}{2}\right\rfloor R + \left\lfloor\frac{m}{2}\right\rfloor r\right)}{Rr} &= \frac{\left(\frac{m}{2}R + \frac{m}{2}r\right)\left(\frac{m}{2}R + \frac{m}{2}r\right)}{Rr} = \\ = \frac{m^2}{4}\left(\sqrt{\frac{R}{r}} + \sqrt{\frac{r}{R}}\right) &= m^2\left(1 + \frac{1}{4}\left(\sqrt{\frac{R}{r}} - \sqrt{\frac{r}{R}}\right)^2\right).\end{aligned} \tag{10}$$

Now, suppose that m is odd. Then

$$\begin{aligned}\frac{\left(\left\lfloor\frac{m}{2}\right\rfloor R + \left\lfloor\frac{m+1}{2}\right\rfloor r\right)\left(\left\lfloor\frac{m+1}{2}\right\rfloor R + \left\lfloor\frac{m}{2}\right\rfloor r\right)}{Rr} &= \frac{\left(\frac{m-1}{2}R + \frac{m+1}{2}r\right)\left(\frac{m+1}{2}R + \frac{m-1}{2}r\right)}{Rr} = \\ = \frac{(m^2-1)(R-r)^2 + 4m^2rR}{4Rr} &= m^2\left(1 + \frac{m^2-1}{4m^2}\left(\sqrt{\frac{R}{r}} - \sqrt{\frac{r}{R}}\right)^2\right).\end{aligned} \tag{11}$$

According to (8), (10) and (11) we arrive at (9).

3. Main Results

In the following theorem we prove the inequality that determines an upper bound for index H in terms of topological index M_1 and graph parameters m, Δ_{e_1} and δ_{e_1}.

Theorem 3.1. *Let G be a simple graph of order n with $m \ge 2$ edges. Then*

$$H \le \frac{2m^2}{M_1}\left(1 + \alpha(m)\left(\sqrt{\frac{\Delta_{e_1}}{\delta_{e_1}}} - \sqrt{\frac{\delta_{e_1}}{\Delta_{e_1}}}\right)^2\right), \tag{12}$$

with equality if $L(G)$ is regular, or $\Delta_{e_1} = d(e_1) + 2 = \cdots = d(e_k) + 2 \ge d(e_{k+1}) + 2 = \cdots = d(e_m) + 2 = \delta_{e_1}$, for $k = \left\lfloor\frac{m}{2}\right\rfloor$ or $k = \left\lfloor\frac{m+1}{2}\right\rfloor$.

Proof. For $a_i = d(e_i) + 2$, $i = 1, 2, \ldots, m$, $R = \Delta_{e_1} = d(e_1) + 2$ and $r = \delta_{e_1} = d(e_m) + 2$, the inequality (9) transforms into

$$\sum_{i=1}^{m}(d(e_i)+2)\sum_{i=1}^{m}\frac{1}{d(e_i)+2} \le m^2\left(1 + \alpha(m)\left(\sqrt{\frac{\Delta_{e_1}}{\delta_{e_1}}} - \sqrt{\frac{\delta_{e_1}}{\Delta_{e_1}}}\right)^2\right).$$

Having in mind (5) the above inequality becomes

$$M_1 \cdot \frac{1}{2}H \le m^2\left(1 + \alpha(m)\left(\sqrt{\frac{\Delta_{e_1}}{\delta_{e_1}}} - \sqrt{\frac{\delta_{e_1}}{\Delta_{e_1}}}\right)^2\right),$$

wherefrom inequality (12) is obtained.

Equality in (8) is attained if $R = a_1 = \cdots = a_m = r$, or if $R = a_1 = \cdots = a_k \geq a_{k+1} = \cdots = a_m = r$ for $k = \left\lfloor \frac{m}{2} \right\rfloor$ or $k = \left\lfloor \frac{m+1}{2} \right\rfloor$. This implies that equality in (12) holds if $L(G)$ is regular, or $\Delta_{e_1} = d(e_1) + 2 = \cdots = d(e_k) + 2 \geq d(e_{k+1}) + 2 = \cdots = d(e_m) + 2 = \delta_{e_1}$ for $k = \left\lfloor \frac{m}{2} \right\rfloor$ or $k = \left\lfloor \frac{m+1}{2} \right\rfloor$. □

Remark 3.2. *Since*

$$H \leq \frac{2m^2}{M_1}\left(1 + \alpha(m)\left(\sqrt{\frac{\Delta_{e_1}}{\delta_{e_1}}} - \sqrt{\frac{\delta_{e_1}}{\Delta_{e_1}}}\right)^2\right) \leq \frac{m^2}{2M_1}\left(\sqrt{\frac{\Delta_{e_1}}{\delta_{e_1}}} + \sqrt{\frac{\delta_{e_1}}{\Delta_{e_1}}}\right)^2 \leq \frac{m^2}{2M_1}\left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2,$$

the inequality (12) *is stronger than* (3).

Corollary 3.3. *Let G be a simple connected graph with n vertices and m ≥ 2 edges. Then*

$$H \leq \frac{n}{2}\left(1 + \alpha(m)\left(\sqrt{\frac{\Delta_{e_1}}{\delta_{e_1}}} - \sqrt{\frac{\delta_{e_1}}{\Delta_{e_1}}}\right)^2\right).$$

Equality is attained if G is regular.

Proof. The above inequality is obtained from (12) and

$$M_1 \geq \frac{4m^2}{n}$$

which was proved in [2]. □

Corollary 3.4. *Let G be a simple connected graph with n vertices and m ≥ 2 edges. Then*

$$H \leq \frac{2m}{\delta_{e_1}}\left(1 + \alpha(m)\left(\sqrt{\frac{\Delta_{e_1}}{\delta_{e_1}}} - \sqrt{\frac{\delta_{e_1}}{\Delta_{e_1}}}\right)^2\right).$$

Equality is attained if L(G) is regular.

By a similar procedure as in case of Theorem 3.1, the following can be proved:

Theorem 3.5. *Let G be a simple connected graph with n vertices and m edges. If m ≥ 3, then*

$$H \leq \frac{2}{\Delta_{e_1}} + \frac{2(m-1)^2}{M_1 - \Delta_{e_1}}\left(1 + \alpha(m-1)\left(\sqrt{\frac{\Delta_{e_2}}{\delta_{e_1}}} - \sqrt{\frac{\delta_{e_1}}{\Delta_{e_2}}}\right)^2\right),$$

with equality if $\Delta_{e_2} = d(e_2) + 2 = \cdots = d(e_m) + 2 = \delta_{e_1}$, *or* $\Delta_{e_2} = d(e_1) + 2 = \cdots = d(e_k) + 2 \geq d(e_{k+1}) + 2 = \cdots = d(e_m) + 2 = \delta_{e_1}$ *for* $k = \left\lfloor \frac{m-1}{2} \right\rfloor$ *or* $k = \left\lfloor \frac{m}{2} \right\rfloor$.

If m ≥ 3, then

$$H \leq \frac{2}{\delta_{e_1}} + \frac{2(m-1)^2}{M_1 - \delta_{e_1}}\left(1 + \alpha(m-1)\left(\sqrt{\frac{\Delta_{e_1}}{\delta_{e_2}}} - \sqrt{\frac{\delta_{e_2}}{\Delta_{e_1}}}\right)^2\right)$$

with equality if $\Delta_{e_1} = d(e_1) + 2 = \cdots = d(e_{m-1}) + 2 = \delta_{e_2}$, *or* $\Delta_{e_1} = d(e_1) + 2 = \cdots = d(e_k) + 2 \geq d(e_{k+1}) + 2 = \cdots = d(e_{m-1}) + 2 = \delta_{e_2}$ *for* $k = \left\lfloor \frac{m-1}{2} \right\rfloor$ *or* $k = \left\lfloor \frac{m}{2} \right\rfloor$.

If $m \geq 4$, then

$$H \leq \frac{2(\Delta_{e_1}+\delta_{e_1})}{\Delta_{e_1}\delta_{e_1}} + \frac{2(m-2)^2}{M_1-\delta_{e_1}-\Delta_{e_1}}\left(1+\alpha(m-2)\left(\sqrt{\frac{\Delta_{e_2}}{\delta_{e_2}}}-\sqrt{\frac{\delta_{e_2}}{\Delta_{e_2}}}\right)^2\right),$$

with equality if $\Delta_{e_2} = d(e_2)+2 = \cdots = d(e_{m-1})+2 = \delta_{e_2}$, or $\Delta_{e_2} = d(e_2)+2 = \cdots = d(e_k)+2 \geq d(e_{k+1})+2 = \cdots = d(e_{m-1})+2 = \delta_{e_2}$, for $k = \left\lfloor \frac{m-2}{2} \right\rfloor$ or $k = \left\lfloor \frac{m-1}{2} \right\rfloor$.

Theorem 3.6. *Let G be a simple connected graph with n vertices and $m \geq 2$ edges. Then*

$$H \leq \frac{X^2}{2m}\frac{\left(\sqrt{\Delta_{e_1}}+\sqrt{\delta_{e_1}}\right)^2}{\sqrt{\Delta_{e_1}\delta_{e_1}}}, \tag{13}$$

with equality if $L(G)$ is regular.

Proof. For $p_i = \frac{\frac{1}{\sqrt{d(e_i)+2}}}{\sum_{i=1}^m \frac{1}{\sqrt{d(e_i)+2}}}$, $a_i = \sqrt{d(e_i)+2}$, $i = 1,2,\ldots,m$, $R = \sqrt{\Delta_{e_1}} = \sqrt{d(e_1)+2}$ and $r = \sqrt{\delta_{e_1}} = \sqrt{d(e_m)+2}$, the inequality (7) becomes

$$\frac{m}{\sum_{i=1}^m \frac{1}{\sqrt{d(e_i)+2}}}\cdot\frac{\sum_{i=1}^m \frac{1}{d(e_i)+2}}{\sum_{i=1}^m \frac{1}{\sqrt{d(e_i)+2}}} \leq \frac{1}{4}\left(\sqrt{\frac{\sqrt{\Delta_{e_1}}}{\sqrt{\delta_{e_1}}}}+\sqrt{\frac{\sqrt{\delta_{e_1}}}{\sqrt{\Delta_{e_1}}}}\right)^2.$$

According to (5) the above inequality transforms into

$$\frac{m}{X}\cdot\frac{\frac{1}{2}H}{X} \leq \frac{1}{4}\frac{(\sqrt{\Delta_{e_1}}+\sqrt{\delta_{e_1}})^2}{\sqrt{\Delta_{e_1}\delta_{e_1}}},$$

wherefrom inequality (13) is obtained. □

Similarly, the following theorem can be proved.

Theorem 3.7. *Let G be a simple connected graph with n vertices and m edges. If $m \geq 3$, then*

$$H \leq \frac{2}{\Delta_{e_1}} + \frac{\left(X-\frac{1}{\sqrt{\Delta_{e_1}}}\right)^2}{2(m-1)}\cdot\frac{\left(\sqrt{\Delta_{e_2}}+\sqrt{\delta_{e_1}}\right)^2}{\sqrt{\Delta_{e_2}\delta_{e_1}}},$$

with equality if $\Delta_{e_2} = d(e_2)+2 = \cdots = d(e_m)+2 = \delta_{e_1}$.

If $m \geq 3$ then

$$H \leq \frac{2}{\delta_{e_1}} + \frac{\left(X-\frac{1}{\sqrt{\delta_{e_1}}}\right)^2}{2(m-1)}\cdot\frac{\left(\sqrt{\Delta_{e_1}}+\sqrt{\delta_{e_2}}\right)^2}{\sqrt{\Delta_{e_1}\delta_{e_2}}},$$

with equality if $\Delta_{e_1} = d(e_1)+2 = \cdots = d(e_{m-1})+2 = \delta_{e_2}$.

If $m \geq 4$, then

$$H \leq \frac{2(\Delta_{e_1}+\delta_{e_1})}{\Delta_{e_1}\delta_{e_1}} + \frac{\left(X-\frac{1}{\sqrt{\Delta_{e_1}}}-\frac{1}{\sqrt{\delta_{e_1}}}\right)^2}{2(m-2)}\cdot\frac{\left(\sqrt{\Delta_{e_2}}+\sqrt{\delta_{e_2}}\right)^2}{\sqrt{\Delta_{e_2}\delta_{e_2}}},$$

with equality if $\Delta_{e_2} = d(e_2)+2 = \cdots = d(e_{m-1})+2 = \delta_{e_2}$.

In the next theorem we establish a lower bound for the index H in terms of X and graph parameters m, Δ_{e_1} and δ_{e_1}.

Theorem 3.8. *Let G be a simple connected graph with n vertices and $m \geq 2$ edges. Then*

$$H \geq \frac{2X^2}{m} + \frac{\left(\sqrt{\Delta_{e_1}} - \sqrt{\delta_{e_1}}\right)^2}{\Delta_{e_1}\delta_{e_1}}. \tag{14}$$

Equality is attained if $L(G)$ is regular, or $\frac{1}{\sqrt{d(e_2)+2}} = \frac{1}{\sqrt{d(e_3)+2}} = \cdots = \frac{1}{\sqrt{d(e_{m-1})+2}} = d$, $\frac{1}{\sqrt{d(e_1)+2}} = d - S$ and $\frac{1}{\sqrt{d(e_m)+2}} = d + S$, where d and S are real numbers so that $d > S \geq 0$.

Proof. For $a_i = \frac{1}{\sqrt{d(e_i)+2}}$, $i = 1, 2, \ldots, m$, $R = \frac{1}{\sqrt{\delta_{e_1}}}$ and $r = \frac{1}{\sqrt{\Delta_{e_1}}}$, the inequality (6) becomes

$$m\sum_{i=1}^{m} \frac{1}{d(e_i)+2} - \left(\sum_{i=1}^{m} \frac{1}{\sqrt{d(e_i)+2}}\right)^2 \geq \frac{m}{2}\left(\frac{1}{\sqrt{\delta_{e_1}}} - \frac{1}{\sqrt{\Delta_{e_1}}}\right)^2.$$

According to (5) and the above we obtain

$$\frac{m}{2}H - X^2 \geq \frac{m}{2}\frac{\left(\sqrt{\Delta_{e_1}} - \sqrt{\delta_{e_1}}\right)^2}{\Delta_{e_1}\delta_{e_1}},$$

wherefrom (14) is obtained. □

Corollary 3.9. *Let G be a simple connected graph with n vertices and $m \geq 2$ edges. Then*

$$H \geq \frac{2m^2}{M_1} + \frac{\left(\sqrt{\Delta_{e_1}} - \sqrt{\delta_{e_1}}\right)^2}{\Delta_{e_1}\delta_{e_1}}, \tag{15}$$

with equality if $L(G)$ is regular.

Proof. Let $p = (p_i)$, $i = 1, 2, \ldots, m$, be a sequence of positive real numbers, and $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, \ldots, m$ non-negative real number sequences of similar monotonicity, then (see for example [13])

$$\sum_{i=1}^{m} p_i \sum_{i=1}^{m} p_i a_i b_i \geq \sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} p_i b_i. \tag{16}$$

If $a = (a_i)$ and $b = (b_i)$ are of opposite monotonicity, then the opposite inequality in (16) is valid. For $p_i = a_i = \sqrt{d(e_i)+2}$, $b_i = \frac{1}{\sqrt{d(e_i)+2}}$, $i = 1, 2, \ldots, m$, we obtain

$$\left(\sum_{i=1}^{m} \sqrt{d(e_i)+2}\right)^2 \leq mM_1. \tag{17}$$

For $p_i = \sqrt{d(e_i)+2}$, $a_i = b_i = \frac{1}{\sqrt{d(e_i)+2}}$, $i = 1, 2, \ldots, m$, from (16) we obtain

$$\left(\sum_{i=1}^{m} \sqrt{d(e_i)+2}\right) \cdot X \geq m^2. \tag{18}$$

Now, according to (17) and (18), we have that

$$\frac{2X^2}{m} \geq \frac{2m^2}{M_1}\,.$$

From the above and (14), the inequality (15) is obtained. □

Remark 3.10. *Since*

$$\left(\sqrt{\Delta_{e_1}} - \sqrt{\delta_{e_1}}\right)^2 \geq 0\,,$$

the inequality (15) *is stronger than* (4).

By a similar procedure as in case of Theorem 3.8, the following can be proved:

Theorem 3.11. *Let G be a simple connected graph with n vertices and m edges. If* $m \geq 3$, *then*

$$H \geq \frac{2}{\Delta_{e_1}} + \frac{2\left(X - \frac{1}{\sqrt{\Delta_{e_1}}}\right)^2}{m-1} + \frac{\left(\sqrt{\Delta_{e_2}} - \sqrt{\delta_{e_1}}\right)^2}{\Delta_{e_2}\delta_{e_1}}\,,$$

with equality if $\Delta_{e_2} = d(e_2) + 2 = \cdots = d(e_m) + 2 = \delta_{e_1}$.

If $m \geq 3$, *then*

$$H \geq \frac{2}{\delta_{e_1}} + \frac{2\left(X - \frac{1}{\sqrt{\delta_{e_1}}}\right)^2}{m-1} + \frac{\left(\sqrt{\Delta_{e_1}} - \sqrt{\delta_{e_2}}\right)^2}{\Delta_{e_1}\delta_{e_2}}\,,$$

with equality if $\Delta_{e_1} = d(e_1) + 2 = \cdots = d(e_{m-1}) + 2 = \delta_{e_2}$.

If $m \geq 4$, *then*

$$H \geq \frac{2(\Delta_{e_1} + \delta_{e_1})}{\Delta_{e_1}\delta_{e_1}} + \frac{2\left(X - \frac{1}{\sqrt{\Delta_{e_1}}} - \frac{1}{\sqrt{\delta_{e_1}}}\right)^2}{m-2} + \frac{\left(\sqrt{\Delta_{e_2}} - \sqrt{\delta_{e_2}}\right)^2}{\Delta_{e_2}\delta_{e_2}}\,,$$

with equality if $\Delta_{e_2} = d(e_2) + 2 = \cdots = d(e_{m-1}) + 2 = \delta_{e_2}$.

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