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KG-SOMBOR ENERGY OF GRAPHS WITH SELF LOOPS

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Abstract. Let $G = (V, E)$ be a connected graph. A topological invariant named KG-Sombor index was introduced by V. R. Kulli, defined as $KG = KG(G) = \sum_{ue} \sqrt{d(u)^2 + d(e)^2}$, where $\sum_{ue}$ indicates summation over vertices $u \in V(G)$ and the edges $e \in E(G)$ that are incident to u. In this paper, we extend the KG-Sombor index of simple graphs to graph with self loops. We study some properties of KG-Sombor eigenvalues and few bounds for KG-Sombor energy of graphs with self loops and KG-Sombor characteristic polynomial of graphs with self loops.

Let $G = (V, E)$ be a simple, finite, undirected and connected graph. The order and size of G is given by $|V| = n$ and $|E| = m$ respectively. The degree of a vertex v in a graph G, denoted by $\deg(v)$ is the number of edges incident on the vertex v. The concept, energy of a graph was coined by I. Gutman in 1978 as the sum of the absolute values of all the eigenvalues of $A(G)$ of a graph denoted by $E(G)$. This definition is a general formula to calculate total π-electron energies of conjugated hydrocarbon molecules which was calculated by Erich Huckel in Huckel molecular orbital theory.
For more on energy of graphs, one can refer [1, 4, 7, 8].
A topological graph index, also called a molecular descriptor, is a mathematical formula that can be applied to any graph which models some molecular structure. Topological indices are mainly categorized into two types: namely degree-based indices and distance-based indices. Some of the degree-based indices are first Zagreb index, second Zagreb index, forgotten index, Randic index, harmonic index, etc. Recently, Gutman et al. [6] defined new degree-based indices, called the Sombor index, which is one of the trending research area of graph theory. Sombor index is defined as,

$$SO = SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2}.$$

For further information on the Sombor index, see references [2, 3, 5, 8].
A vertex-edge variant of the Sombor index was introduced by V. R. Kulli et al. [10], which is defined as

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$$KG = KG(G) = \sum_{ue} \sqrt{d(u)^2 + d(e)^2}, \tag{0.1}$$

where $\sum\limits_{ue}$ indicates summation over vertices $u \in V(G)$ and the edges $e \in E(G)$ that are incident to u.
Since the edge $e = uv$ is incident to both the vertices u and v, we can also express equation (0.1) as

$$KG(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + [d(u) + d(v) - 2]^2} + \sqrt{d(v)^2 + [d(u) + d(v) - 2]^2}.$$

The readers are directed to refer [9, 11, 13, 14, 15] for more information on KG-Sombor index.
Let $S \in V(G)$ and $|S| = k$. Let G_S be the graph obtained from the simple graph G, by attaching a self-loop to each of its vertices belonging to S. Let $X(G_S)$ and $d_i(G_S)$ represent edge set of G_S and degree of vertex v_i in G_S, for $1 \leq i \leq n$ respectively.
In this paper, we define KG-Sombor matrix for graph with self loops as $KG(G_S) = d_{ij}$, where

$$d_{ij} = \begin{cases} \sqrt{(d(u)^2 + [d(u) + d(v) - 2])^2} + \sqrt{d(v)^2 + [d(u) + d(v) - 2])^2}, & \text{if } u \sim v \\ 0, & \text{if } u \nsim v \\ 2\sqrt{(d(u)^2 + [2d(u) - 2])^2}, & \text{if } u \in S \\ 0, & \text{if } u \notin S. \end{cases}$$

Let $\sigma_1(G_S), \sigma_2(G_S), \ldots, \sigma_n(G_S)$ be the eigenvalues of $KG(G_S)$.
The KG-Sombor energy of graphs with self loops is defined as,

$$EKG(G_S) = \sum_{i=1}^{n} \left| \sigma_i(G_S) - \frac{2 \sum\limits_{\substack{u=v \\ u \in S}} N}{n} \right|,$$

where, $N = \sqrt{(d(u)^2 + [2d(u) - 2])^2}$.
Let $k_i = \left| \sigma_i(G_S) - \frac{2 \sum\limits_{\substack{u=v \\ u \in S}} N}{n} \right|$, $i = 1, 2, \ldots, n$ denote the auxiliary eigenvalues of $KG(G_S)$.

Lemma 0.1. *Let $x_1, x_2, \ldots, x_n$ and $y_1, y_2, \ldots, y_n$ be real numbers. If there exist real constants x, y, X and Y such that for each i, $i = 1, 2, \ldots, n, x \leq x_i \leq X$ and $y \leq y_i \leq Y$, then $\left| n \sum\limits_{i=1}^{n} x_i y_i - \sum\limits_{i=1}^{n} x_i \sum\limits_{i=1}^{n} y_i \right| \leq \alpha(n)(X - x)(Y - y)$, where $\alpha(n) = n[\frac{n}{2}]\left(1 - \frac{1}{n}[\frac{n}{2}]\right)$. The equality holds if and only if $a_i = a_j$ and $b_i = b_j$ for all $1 \leq i, j \leq n$.*

Lemma 0.2. *Suppose p, q are non-negative integers, and suppose A, B, C, D are respectively $p \times p$, $p \times q$, $q \times p$, and $q \times q$ matrices of complex numbers. Let*

$M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ *so that* M *is a* $(p+q) \times (p+q)$ *matrix. If* A *is invertible, then* $det(M) = det(A)det(D - CA^{-1}B)$.

1. KG-Sombor eigenvalues of (G_S)

Theorem 1.1. *Let* $G = (V, X)$ *be a graph with* $|V| = n$ *and* $|X| = m$*. Then, the eigenvalues* $\sigma_1(G_S), \sigma_2(G_S), \ldots, \sigma_n(G_S)$ *of* $KG(G_S)$ *satisfy,*

(1) $\sum\limits_{i=1}^{n} \sigma_i(G_S) = 2 \sum\limits_{\substack{u=v \\ u \in S}} N$.

(2) $\sum\limits_{i=1}^{n} \sigma_i^2(G_S) = 2(\sum\limits_{u \neq v} M^2 + 2 \sum\limits_{\substack{u=v \\ u \in S}} N^2)$.

Proof. 1. We have,

$$\begin{aligned} \sum_{i=1}^{n} \sigma_i(G_S) &= \sum_{i=1}^{n} [KG(G_S)] \\ &= \sum_{u \in S} 2\sqrt{d(u)^2 + [2d(u) - 2]^2} \\ &= 2 \sum_{\substack{u=v \\ u \in S}} N. \end{aligned}$$

2. Also,

$$\begin{aligned} \sum_{i=1}^{n} \sigma_i^2(G_S) = 2 &\left\{ \sqrt{d(u)^2 + [d(u) + d(v) - 2]^2} + \sqrt{d(v)^2 + [d(u) + d(v) - 2]^2} \right\} \\ &+ \sum_{\substack{u=v \\ u \in S}} (2N)^2 \\ &= 2 \left(\sum_{u \neq v} M^2 + 2 \sum_{\substack{u=v \\ u \in S}} N^2 \right). \end{aligned}$$

□

Theorem 1.2. *Let* $G = (V, X)$ *be a graph with* $|V| = n$ *and* $|X| = m$*. Then, the auxiliary eigenvalues* $k_1(G_S), k_2(G_S), \ldots, k_n(G_S)$ *of* $KG(G_S)$ *satisfy,*

(1) $\sum\limits_{i=1}^{n} k_i = 0$.

(2) $\sum\limits_{i=1}^{n} k_i^2 = \dfrac{2 \left\{ n \sum\limits_{u \neq v} M^2 + 2n \sum\limits_{\substack{u=v \\ u \in S}} N^2 - 2 \left(\sum\limits_{\substack{u=v \\ u \in S}} N)^2 \right) \right\}}{n}$.

Proof. 1. We have,

$$\sum_{i=1}^{n} k_i = \sum_{i=1}^{n}\left(\sigma_i(G_S) - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right)$$
$$= \sum_{i=1}^{n}\sigma_i(G_S) - \sum_{i=1}^{n}\frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}$$
$$= 0.$$

2. Also,

$$\sum_{i=1}^{n} k_i^2 = \sum_{i=1}^{n}\left(\sigma_i(G_S) - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right)^2$$
$$= \sum_{i=1}^{n}\sigma_i(G_S)^2 + \sum_{i=1}^{n}\left(\frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right)^2 - 2\sum_{i=1}^{n}\sigma_i(G_S)\left(\frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right)$$
$$= \frac{2\left(n\sum\limits_{u\neq v} M^2 + 2n\sum\limits_{\substack{u=v\\u\in S}} N^2 - 2(\sum\limits_{\substack{u=v\\u\in S}} N)^2\right)}{n}$$
$$= P.$$

□

2. Bounds on $KG(G_S)$

Theorem 2.1. *Let $G = (V, X)$ be a graph with $|V| = n$ and $|X| = m$. Then, $EKG(G_S) \leq \sqrt{nP}$.*

Proof. Taking $a_i = 1$ and $b_i = |k_i|$ in Cauchy-Schwarz inequality, we get

$$\left(\sum_{i=1}^{n}|k_i|\right)^2 \leq \left(\sum_{i=1}^{n}1\right)\left(\sum_{i=1}^{n}|k_i|^2\right)$$
$$(EKG(G_S))^2 \leq nP$$
$$EKG(G_S) \leq \sqrt{nP}.$$

□

Theorem 2.2. *Let $G = (V, X)$ be a graph with $S \subseteq G$. Then*
$EKG(G_S) \geq \sqrt{2P + n(n-1)D^{\frac{2}{n}}}$, where $D = |KG(G_S)|$.

Proof. Using arithmetic and geometric mean inequality,

$$\frac{1}{n(n-1)}\sum_{i\neq j}\left|\sigma_i(G_S)-\frac{2\sum\limits_{\substack{u=v\\u\in S}}N}{n}\right|\left|\sigma_j(G_S)-\frac{2\sum\limits_{\substack{u=v\\u\in S}}N}{n}\right|$$

$$\geq\left(\prod_{i\neq j}\left|\sigma_i(G_S)-\frac{2\sum\limits_{\substack{u=v\\u\in S}}N}{n}\right|\left|\sigma_j(G_S)-\frac{2\sum\limits_{\substack{u=v\\u\in S}}N}{n}\right|\right)^{\dfrac{1}{n(n-1)}}$$

$$=\left(\prod_{i\neq j}\left|\sigma_i(G_S)-\frac{2\sum\limits_{\substack{u=v\\u\in S}}N}{n}\right|^{2(n-1)}\right)^{\dfrac{1}{n(n-1)}}$$

$$=\left(\prod_{i\neq j}\left|\sigma_i(G_S)-\frac{2\sum\limits_{\substack{u=v\\u\in S}}N}{n}\right|\right)^{\dfrac{2}{n}}$$

$$=D^{\frac{2}{n}},$$

where $D=|KG(G_S)|$.
Therefore,

$$\sum_{i\neq j}\left|\sigma_i(G_S)-\frac{2\sum\limits_{\substack{u=v\\u\in S}}N}{n}\right|\left|\sigma_j(G_S)-\frac{2\sum\limits_{\substack{u=v\\u\in S}}N}{n}\right|\geq n(n-1)D^{\frac{2}{n}}.$$

Consider,

$$(EKG(G_S))^2=\left(\sum_{i=1}^{n}\left|\sigma_i(G_S)-\frac{2\sum\limits_{\substack{u=v\\u\in S}}N}{n}\right|\right)^2$$

$$=\sum_{i=1}^{n}\left|\sigma_i(G_S)-\frac{2\sum\limits_{\substack{u=v\\u\in S}}N}{n}\right|^2+\sum_{i\neq j}\left|\sigma_i(G_S)-\frac{2\sum\limits_{\substack{u=v\\u\in S}}N}{n}\right|\left|\sigma_j(G_S)-\frac{2\sum\limits_{\substack{u=v\\u\in S}}N}{n}\right|$$

$$\geq\sqrt{P+n(n-1)D^{\frac{2}{n}}}.$$

□

Theorem 2.3. *Let G_S be a connected graph of order $n \geq 2$ and $S \subseteq G$. Then*

$$EKG(G_S) \leq \left(\sigma_1(G_S) - \frac{\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right)$$
$$+\sqrt{(n-1)(P - \sigma_1^2 + (n-1)4\left(\frac{\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right)^2 - 4\frac{\sum\limits_{\substack{u=v\\u\in S}} N}{n}\left(2\sum_{\substack{u=v\\u\in S}} N - \sigma_1(G_s)\right)}.$$

Proof. Applying Cauchy-Schwartz inequality for $(n-1)$ terms,

$$\left(\sum_{i=2}^{n}\left|\sigma_i(G_S) - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|\right)^2 \leq \left(\sum_{i=2}^{n} 1\right)\left(\sum_{i=2}^{n}\left|\sigma_i(G_S) - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|\right)$$

$$\left(EKG(G_S) - \left|\sigma_1(G_S) - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|\right)^2 \leq (n-1)\left(\sum_{i=2}^{n}\sigma_i(G_S)^2 + 4\sum_{i=2}^{n}\left(\frac{\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right)^2 - 4\frac{\sum\limits_{\substack{u=v\\u\in S}} N}{n}\sum_{i=2}^{n}\sigma_i(G_S)\right)$$

$$EKG(G_S) \leq \left(\sigma_1(G_S) - \frac{\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right)$$
$$+\sqrt{(n-1)(P - \sigma_1^2 + (n-1)4\left(\frac{\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right)^2 - 4\frac{\sum\limits_{\substack{u=v\\u\in S}} N}{n}\left(2\sum_{\substack{u=v\\u\in S}} N - \sigma_1(G_s)\right)}.$$

□

Theorem 2.4. *For a graph G_S obtained by adding k self-loops to the graph $G(n,m)$,*
$KG(G_S) \leq \frac{\sqrt{nP}}{2}$.

Proof. $$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\left|\sigma_i - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right| - \left|\sigma_j - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|\right)^2 \geq 0$$

$$n\sum_{i=1}^{n}\left|\sigma_i - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|^2 + n\sum_{j=1}^{n}\left|\sigma_j - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|^2 \geq 2\sum_{i=1}^{n}\left|\sigma_i - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|\sum_{j=1}^{n}\left|\sigma_j - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|$$

$$\implies nP \geq 2(KG(G_S))^2$$

$$\implies KG(G_S) \leq \frac{\sqrt{nP}}{2}.$$

□

Theorem 2.5. *Let $\sigma_1(G_S), \sigma_2(G_S), \ldots, \sigma_n(G_S)$ be the KG-Sombor eigenvalues of the graph G_S containing k self-loops. Then,*

$$EKG(G_S) \geq \sqrt{nP - \frac{n^2}{4}\left(\left|\sigma_1 - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right| - \left|\sigma_n - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|\right)^2}.$$

Proof. Let $\left|\sigma_1 - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|, \left|\sigma_2 - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|, \ldots, \left|\sigma_n - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|$ be a non-increasing arrangement of KG-Sombor eigenvalues of G_S.

On substituting $x_i = y_i = \left|\sigma_i - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|$, $x = y = \left|\sigma_n - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|$ and $X = Y = \left|\sigma_1 - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|$ in lemma 0.1 and noting $\alpha(n) \leq \frac{n^2}{4}$,

$$\left|n\sum_{i=1}^{n}\left|\sigma_i(G_S) - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|^2 - \sum_{i=1}^{n}\left|\sigma_i(G_S) - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|^2\right| \leq \frac{n^2}{4}\left(\left|\sigma_1 - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right| - \left|\sigma_n - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|\right)^2.$$

But,

$$\sum_{i=1}^{n}\left|\sigma_i - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right| = EKG(G_S) \text{ and } \sum_{i=1}^{n}\left|\sigma_i - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|^2 = P. \text{ Now,}$$

$$n(P) - (EKG(G_S))^2 \leq \frac{n^2}{4}\left(\left|\sigma_1 - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right| - \left|\sigma_n - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|\right)^2.$$

$$\Longrightarrow EKG(G_S) \geq \sqrt{nP - \frac{n^2}{4}\left(\left|\sigma_1 - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right| - \left|\sigma_n - \frac{2\sum\limits_{\substack{u=v\\u\in S}} N}{n}\right|\right)^2}.$$

□

3. KG-Sombor Energy of G_S

Theorem 3.1. *For complete graph K_n with $k \geq 1$ self-loops, the KG-Sombor characteristic polynomial $p(x)$ is $\sigma^{k-1}(\sigma + c)^{n-k-1}(\sigma^2 + \sigma(c - ak + ck - cn) + b^2k^2 - ack - ack^2 - b^2kn + ackn)$.*

Proof. For complete graph K_n with $k \geq 1$ self-loops, we have

$$KG((K_n)_S) = \begin{bmatrix} aJ_k & bJ_{k\times(n-k)} \\ bJ_{(n-k)\times k} & c(J-I)_{(n-k)} \end{bmatrix}_n,$$

where J is matrix of all 1's, $a = 2\sqrt{5n^2+2n+1}$,
$b = \sqrt{5n^2-6n+5} + \sqrt{5n^2-10n+5}$, and $c = 2\sqrt{5n^2-18n+17}$.
Let $W = \begin{bmatrix} Y \\ Z \end{bmatrix}$ be an eigenvector of order n, such that vector Y be of order k and vector Z be of order $n-k$. If $\sigma(G_S)$ be a eigenvalue of $KG((K_n)_S)$. Then,

$$[KG((K_n)_S) - \sigma I]\begin{bmatrix} Y \\ Z \end{bmatrix} = \begin{bmatrix} (aJ-\sigma I)Y + (bJ)Z \\ (bJ)Y + (cJ - I(c+\sigma))Z \end{bmatrix}_n. \tag{3.1}$$

Case 1. Let $Y = Y_j = e_1 - e_j$, $j = 2, 3, \dots, k$ and $Z = 0_{n-k\times 1}$. Using equation (3.1), $[aJ - \sigma I]Y_j + 0 = -\sigma Y_j = 0$ then, $\sigma = 0$ is the eigenvalue with multiplicity of at least $k-1$ since there are $k-1$ independent vectors of the form Y_j.
Case 2. Let $Y = 0_k$ and $Z = Z_j = e_1 - e_j$, $j = 2, 3, \dots, n-k$. Using equation (3.1), $0 + (cJ - I(c+\sigma))Z_j = -(c+\sigma)Z_j = 0$ then, $\sigma = -c$ is the eigenvalue with multiplicity of at least $n-k-1$ since there are $n-k-1$ independent vectors of the form Z_j.
Case 3. Let $Y = \frac{b(n-k)}{\sigma - ka} I_k$ and $Z = I_{(n-k)}$. Here, σ denotes root of the equation, $\sigma^2 + \sigma(c - ak + ck - cn) + b^2k^2 - ack - ack^2 - b^2kn + ackn = 0$.
From equation 3.1,

$$\begin{aligned}(bJ)Y_j + (cJ - I(c+\sigma))Z_j &= bJ\left(\frac{b(n-k)}{\sigma - ka}\right)1_k + \{cJ - I(c+\sigma)\}1_{n-k} \\ &= \frac{b^2(n-k)k}{\sigma - ka}1_{n-k} + c(n-k)1_{n-k} - (c+\sigma)1_{n-k} \\ &= \frac{1}{\sigma - ka}\left(\sigma^2 + \sigma(c - ak + ck - cn) + b^2k^2\right. \\ &\quad \left. - \left(ack - ack^2 - b^2kn + ackn\right)\right)1_{n-k}.\end{aligned}$$

So, $\sigma_1 = \frac{ak + cn - c - ck + \sqrt{(c - ak + ck - cn)^2 - 4(b^2k^2 - ack - ack^2 - b^2kn + ackn)}}{2}$ and $\sigma_2 = \frac{ak + cn - c - ck - \sqrt{(c - ak + ck - cn)^2 - 4(b^2k^2 - ack - ack^2 - b^2kn + ackn)}}{2}$ are the eigenvalues with multiplicity of at least one.
The spectrum of $KG((K_n)_S)$ is given by,

$$\begin{pmatrix} 0 & -c & \sigma_1 & \sigma_2 \\ k-1 & n-k-1 & 1 & 1 \end{pmatrix}$$

where, $\sigma_1 = \frac{ak + cn - c - ck + \sqrt{(c - ak + ck - cn)^2 - 4(b^2k^2 - ack - ack^2 - b^2kn + ackn)}}{2}$,
$\sigma_2 = \frac{ak + cn - c - ck - \sqrt{(c - ak + ck - cn)^2 - 4(b^2k^2 - ack - ack^2 - b^2kn + ackn)}}{2}$.
The the KG-Sombor characteristic polynomial $p(x)$ of $KG((K_n)_S)$ is given by,
$\sigma^{k-1}(\sigma + c)^{n-k-1}(\sigma^2 + \sigma(c - ak + ck - cn) + b^2k^2 - ack - ack^2 - b^2kn + ackn)$.
□

Theorem 3.2. *Let $K_{m,n}$ be complete bipartite graph on $m+n$ vertices. The KG-Sombor characteristic polynomial $p(x)$ of $KG((K_{m,n})_S)$ is given by, $\sigma^{n-1}(\sigma - a)^{m-1}(\sigma^2 - a\sigma - mnb^2)$.*

Proof. For complete bipartite graph $K_{m,n}$ with $k = m$ self-loops, we have

$$[KG((K_{m,n})_S) - \sigma I] = \begin{bmatrix} [a-\sigma I]_m & bJ_{m\times n} \\ bJ_{n\times m} & -\sigma I_n \end{bmatrix}_{m+n},$$

where J is matrix of all 1's and $a = 2\sqrt{(n+2)^2 + (2n+2)^2}$,
$b = \sqrt{(n+2)^2 + (m+n)^2} + \sqrt{m^2 + (m+n)^2}$.
Since block $A = [a - \sigma I]_m$ is invertible, by lemma (0.2), we have $|KG((K_{m,n})_S) - \sigma I| = |[a-\sigma I]_m||-\sigma I_n - bJ_{n\times m}[a-\sigma I]_m^{-1} bJ_{m\times n}|$.
On simplifying, we obtain
$|KG((K_{m,n})_S) - \sigma I| = (a-\sigma)^m(-\sigma)(\sigma)^{n-2}\left(-\sigma - \frac{mnb^2}{a-\sigma}\right)$.
The KG-Sombor characteristic polynomial $p(x)$ of $KG((K_{m,n})_S)$ is given by

$$(\sigma)^{n-1}(\sigma - a)^{m-1}(\sigma^2 - a\sigma - mnb^2).$$

The spectrum of $KG((K_{m,n})_S)$ is given by

$$\begin{pmatrix} 0 & a & \sigma_1 & \sigma_2 \\ n-1 & m-1 & 1 & 1 \end{pmatrix}$$

where, $\sigma_1 = \dfrac{a + \sqrt{a^2 + 4mnb^2}}{2}$ and $\sigma_2 = \dfrac{a - \sqrt{a^2 + 4mnb^2}}{2}$.

□

Theorem 3.3. *For star $K_{1,n-1}$ with $k = 1$ self-loop at the central vertex, the KG-Sombor characteristic polynomial $p(x)$ is $\sigma^{n-k-1}(\sigma - 10)^{k-2}(\sigma^3 - \sigma^2(a+10) + \sigma(10a - b^2k + d^2k - d^2n + b^2) + 10d^2n - 10d^2k)$.*

Proof. For star $K_{1,n-1}$ with $k = 1$ self-loop at the central vertex, we have

$$[KG((K_{1,n-1})_S) - \sigma I] = \begin{bmatrix} (a-\sigma)I_1 & bJ_{1\times(k-1)} & dJ_{1\times(n-k)} \\ bJ_{k-1\times 1} & (10-\sigma)I_{k-1} & 0_{k-1\times(n-k)} \\ dJ_{n-k\times 1} & 0_{n-k\times k-1} & -\sigma I_{n-k} \end{bmatrix}_n,$$

where $a = 2\sqrt{5n^2 + 2n + 1}$, $b = \sqrt{2n^2 + 6n + 5} + \sqrt{n^2 + 4n + 13}$ and
$d = \sqrt{2n^2 + 2n + 1} + \sqrt{1 + n^2}$.

Let $W = \begin{bmatrix} X \\ Y \\ Z \end{bmatrix}$ be an eigenvector of order n, such that such that vector X be of order 1, vector Y be of order $k-1$ and vector Z be of order $n-k$. If $\sigma(G_S)$ is a eigenvalue of $KG((K_{1,n-1})_S)$, then

$$[KG((K_{1,n-1})_S) - \sigma I]\begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} (a-\sigma)I_1X_1 + bJ_{1\times(k-1)}Y_{k-1} + dJ_{1\times(n-k)}Z_{n-k} \\ bJ_{k-1\times 1}X_1 + (10-\sigma)I_{k-1}Y_{k-1} + 0_{k-1\times(n-k)}Z_{n-k} \\ dJ_{n-k\times 1}X_1 + 0_{n-k\times k-1}Y_{k-1} - \sigma I_{n-k}Z_{n-k} \end{bmatrix}_n \tag{3.2}$$

Case 1. Let $X = 0_1$, $Y = 0_{k-1}$ and $Z = Z_j = e_1 - e_j$, $j = 2, 3, \ldots, n-k$. Using equation (3.2), $[-\sigma I]Z_j$, then $\sigma = 0$ is the eigenvalue with multiplicity of at least $n-k-1$ since there are $n-k-1$ independent vectors of the form Z_j.

Case 2. Let $X = 0_1$, $Y = Y_j = e_1 - e_j$, $j = 2, 3, \ldots, k-1$ and $Z = 0_{n-k}$. Using equation (3.2), $((10J - \sigma)I)Y_j$, then $\sigma = 10$ is the eigenvalue with multiplicity of at least $k-2$ since there are $k-2$ independent vectors of the form Y_j.
Case 3. Let $X = 1_1$, $Y = \frac{b}{\sigma-10} I_{(k-1)}$ and $Z = \frac{d}{\sigma} I_{n-k}$.
Here, σ denotes root of the equation $\sigma^3 - \sigma^2(a+10) + \sigma(10a - b^2k + d^2k - d^2n + b^2) + 10d^2n - 10d^2k = 0$.
From equation (3.2),

$$(a - \sigma 1_1)1_1 + bJ_{1\times k-1}\frac{b}{\sigma - 10}I_{k-1} + dJ_{1\times n-k}\frac{d}{\sigma}I_{n-k}$$
$$= (a-\sigma) + \frac{b^2}{\sigma-10}(k-1) + \frac{d^2}{\sigma}(n-k)1_1$$
$$= \frac{1}{\sigma(\sigma-10)}\left(\sigma^3 - \sigma^2(a+10) + \sigma(10a - b^2k + d^2k - d^2n + b^2) + 10d^2n - 10d^2k\right)1_1.$$

Thus, the KG-Sombor characteristic polynomial of $KG((K_{1,n-1})_S)$ is given by
$\sigma^{n-k-1}(\sigma-10)^{k-2}(\sigma^3-\sigma^2(a+10)+\sigma(10a-b^2k+d^2k-d^2n+b^2)+10d^2n-10d^2k)$. □

Theorem 3.4. *The KG-Sombor characteristic polynomial* $p(x)$ *of star* $K_{1,n-1}$ *with* $k \geq 1$ *self-loops for pendant vertices is* $\sigma^{n-k-1}(\sigma - 10)^{k-1}(\sigma^3 - 10\sigma^2 - \sigma(ka^2 + (n-k-1)b^2 - 10(n-k-1)b^2$.

Proof. For star $K_{1,n-1}$ with $k \geq 1$ self-loops for pendant vertices, we have

$$[KG((K_{1,n-1})_S) - \sigma I] = \begin{bmatrix} (0-\sigma)I_1 & aJ_{1\times k} & bJ_{1\times(n-k-1)} \\ aJ_{k\times 1} & (10-\sigma)I_{k\times k} & 0_{k\times(n-k-1)} \\ bJ_{n-k-1\times 1} & 0_{n-k-1\times k} & -\sigma I_{n-k-1} \end{bmatrix}_{n\times n}, \quad (3.3)$$

where $a = \sqrt{(n-1)^2 + n^2} + \sqrt{9+n^2}$, $b = \sqrt{(n-1)^2 + (n-2)^2} + \sqrt{1+(n-2)^2}$.
Step 1: On replacing R_i by $R_i - R_{i-1}$, for $i = 3, \ldots, k-1, k, k+2, \ldots, n$ and replacing C_i by $C_i + C_{i-1} + \cdots + C_{k+1}$, for $i = n, n-1, \ldots, k+1$ and C_j by $C_j + C_{j-1} + \cdots + C_2$, for $j = k, k-1, \ldots, 2$ in equation (3.3) a new determinant say $det(D)$ is obtained.
Step 2: On expanding $det(D)$ along the rows from R_3 to R_k and from R_{k+2} to R_n it reduces to,

$$\sigma^{n-k-1}(\sigma-10)^{k-1}\begin{vmatrix} -\sigma & ka & (n-k-1)b \\ a & 10-\sigma & 0 \\ b & 0 & -\sigma \end{vmatrix}. \quad (3.4)$$

On simplifying equation (3.4), we obtain the KG-Sombor characteristic polynomial $p(x)$ of $KG((K_{1,n-1})_S) = \sigma^{n-k-1}(\sigma-10)^{k-1}(\sigma^3 - 10\sigma^2 - \sigma(ka^2 + (n-k-1)b^2 - 10(n-k-1)b^2$. □

Observations: For path P_n,

- let P_{n1}, P_{n2}, P_{n3} denote the paths with self loop at the end vertex, the vertex whose one of the neighbouring vertex has degree 1 and the other has degree 2, the vertex whose both neighbouring vertices have degree 2 respectively.

  Then, we have $EKG(P_{n1}) \leq EKG(P_{n3}) \leq EKG(P_{n2})$.

- Whenever n is odd, there exists exactly one zero eigenvalue for path P_{n2}.

For $3 \leq n \leq 15$, we have computed the KG-Sombor energy of P_{n1}, P_{n2}, and P_{n3}, as indicated in table (1). Additionally, a graph representing the change in $EKG(P_{n1}), EKG(P_{n2})$, and $EKG(P_{n3})$ has been shown (1).

TABLE 1. $EKG(P_{n1})$, $EKG(P_{n2})$ and $EKG(P_{n3})$

Number of vertices	P_{n1}	P_{n2}	P_{n3}
P3	22.3855	32.0284	-
P4	29.2725	37.1494	-
P5	36.2211	44.1208	42.5768
P6	43.659	50.3647	49.273
P7	50.5031	57.8073	56.3693
P8	58.0456	64.2536	62.9865
P9	64.8806	71.8242	70.5158
P10	72.437	78.3813	77.3777
P11	79.2876	85.9903	84.7809
P12	86.832	92.6207	91.7717
P13	93.7039	100.2346	99.1019
P14	101.2293	106.9194	106.1677
P15	108.1231	114.5246	113.4528

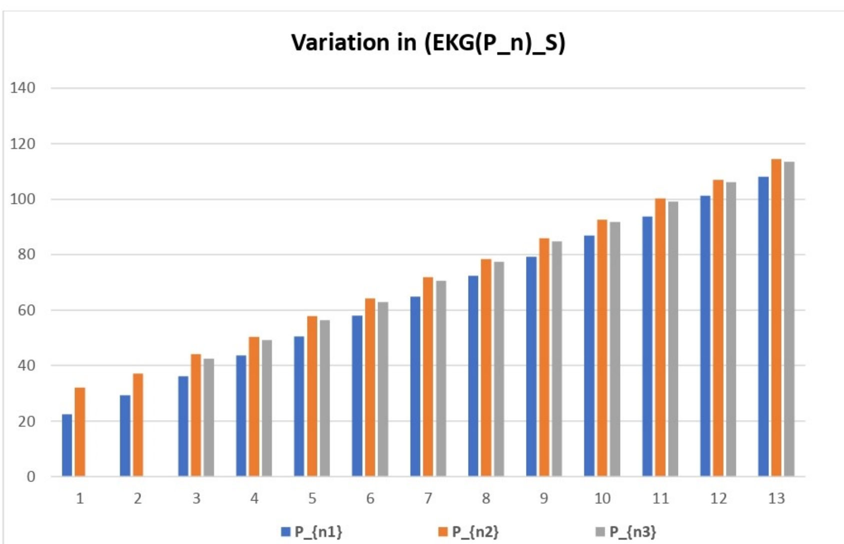

FIGURE 1. Variation in $(EKG(P_n)_S)$

4. Conclusion

In this work, we have computed the KG-Sombor energy of graphs with self loops. Here, we note that whenever the number the self loops is zero, all the results reduces to the case of simple graphs. We have got the expressions for KG-Sombor eigenvalues, bounds on KG-Sombor energy and also computed KG-Sombor characteristic polynomials of complete graphs, complete bipartite graphs, star and observed the variation in KG-Sombor energy of paths with self loops on various positions.

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