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A Note on the Computation of Revised (Edge–)Szeged Index in Terms of Canonical Isometric Embedding*

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Abstract

Motivated by the computation formula of Wiener index in terms of canonical isometric embedding, we deduce computation formulas for the revised (edge-) Szeged index. The revised (edge-)Szeged index for a vertex-edge-weighted graph are thus introduced. We also obtain some properties of the equivalent relation θ^* and the revised (edge-)Szeged index. Finally, we calculate the revised (edge-) Szeged indices for some specific graphs, as examples.

1 Introduction

All graphs in this paper are assumed to be finite, simple and undirected, unless pointed out specifically. We refer the reader to [2] for terminology and notation unexplained here.

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, the *distance* $d_G(u,v)$ counts the minimum number of edges of the path connecting u and v in G. For $u \in V(G)$ and $f \in E(G)$, the *distance* $d_G(u,f)$ counts the minimum number of edges of the path connecting u and f in G. It is naturally to consider partitions of $E(G)$ with respect to an edge $e = uv \in E(G)$ involved with several sets defined below:

$$N_u(e|G) = \{w \in V : d_G(u,w) < d_G(v,w)\},$$

$$N_0(e|G) = \{w \in V : d_G(u,w) = d_G(v,w)\},$$

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$$M_u(e|G) = \{f \in E : d_G(u,f) < d_G(v,f)\},$$
$$M_0(e|G) = \{f \in E : d_G(u,f) = d_G(v,f)\}.$$

Let $n_u(e|G)$, $n_0(e|G)$, $m_u(e|G)$ and $m_0(e|G)$ denote the cardinality of $N_u(e|G)$, $N_0(e|G)$, $M_u(e|G)$ and $M_0(e|G)$, respectively. Note that $u \in N_u(e|G)$ and $e \in M_o(e|G)$. Omit the constraint $|G$ if not necessary.

For two graphs G and G', a map ϕ from $V(G)$ to $V(G')$ is isometric if for all $u, v \in V(G)$, $d_G(u,v) = d_{G'}(\phi(u), \phi(v))$. Attempting to characterize the isometric subgraphs of hypercubes, Djoković [5] introduced an equivalent relation θ on partial cubes, saying that for $e = uv$, $e' = u'v' \in E(G)$, $e\theta e'$ if and only if $d_G(u,u') + d_G(v,v') \neq d_G(u,v') + d_G(v,u')$. Before long, Graham and Winkler [6] generalized the equivalent relation θ into its transitive closure θ^*, which is suitable for all graphs. Moreover, they define the canonical isometric embedding through it, which maps G to the product of a series quotient graphs of G isometrically.

First, recall the definition of the Cartesian product of graphs. In a graph $G = G_1 \Box \cdots \Box G_k$, $u, v \in V(G)$ are adjacent if and only if for some i, u_i is adjacent to v_i in G_i and for any $j \neq i$, $u_j = v_j$. Also note that $d_G(u,v) = \sum_{j=1}^{k} d_{G_j}(u_j, v_j)$.

Denote the equivalent classes of θ^* by $\mathfrak{E} = \{E_1, \cdots, E_k\}$ throughout this paper. Let G_i be the graphs formed from G by deleting E_i and $C_1^i, \cdots, C_{m_i}^i$ be the connected components of G_i. Construct the graphs G_i^* with vertex set $V(G_i^*) = \{C_1^i, \cdots, C_{m_i}^i\}$ and the vertices C_j^i and $C_{j'}^i$ are adjacent if and only if some edge in E_i joins a vertex in C_j^i to a vertex in $C_{j'}^i$. Define maps $\alpha_i : V(G) \to V(G_i^*)$, where $v \in \alpha_i(v)$. Then the canonical isometric representation $\alpha : V(G) \to V(G^*) = V(\Box_{i=1}^k G_i^*)$, where $\alpha(v) = (\alpha_1(v), \cdots, \alpha_k(v))$, is well defined and isometric. For more results on θ and θ^*, see [13].

The *Wiener index* of a graph G is defined as $W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)$. In [11], through the equivalent relation θ, an expansion form of the Wiener index for partial cubes has been deduced: $W(G) = \sum_{e=uv \in E(G)} n_u(e) n_v(e)$. A computation formula of the Wiener index for all graphs also appeared in [10], utilizing the equivalent relation θ^*. We refer the reader to [9,13] for similar results of other indices and [14,15,18] for more information about the Wiener index and the edge-Wiener index.

Motivated by the symmetry expansion form of Wiener index, Gutman [7] introduced graph invariants *Szeged index* defined by $Sz(G) = \sum_{e=uv \in E(G)} n_u(e) n_v(e)$. and [8] the *edge-Szeged index* $Sz_e(G) = \sum_{e=uv \in E(G)} m_u(e) m_v(e)$. Shortly afterwards, Randić [16] raised a modified version of the Szeged index, i.e., the *revised Szeged index.* The *revised Szeged index* of a connected graph G is defined as

$$Sz^*(G) = \sum_{e=uv\in E(G)} (n_u(e) + \frac{1}{2}n_0(e))(n_v(e) + \frac{1}{2}n_0(e)).$$

There is an edge version of the revised Szeged index, the *revised edge-Szeged index*, which is defined as

$$Sz_e^*(G) = \sum_{e=uv\in E(G)} (m_u(e) + \frac{1}{2}m_0(e))(m_v(e) + \frac{1}{2}m_0(e)).$$

There are lots of results about the (edge-)Szeged index and the revised (edge-)Szeged index; see [1,3,4,8]. This paper will give expansion formulas of the revised (edge-) Szeged indices.

We list the necessary notions and lemmas in next section, prove our main results in section 3, and end with two examples in the final section.

2 Preliminaries

Let $G_{\omega,\sigma} = (G, \omega, \sigma)$ be a vertex-edge-weighted graph, which is the graph G with weights $\omega : V(G) \to \mathbb{R}^+$ and $\sigma : E(G) \to \mathbb{R}^+$. Moreover, with respect to $e = uv \in E(G) = E(G_{\omega,\sigma})$, define

$$\begin{aligned}
N_u(e|G_{\omega,\sigma}) &= N_u(e|G),\\
N_0(e|G_{\omega,\sigma}) &= N_0(e|G),\\
M_u(e|G_{\omega,\sigma}) &= M_u(e|G),\\
M_0(e|G_{\omega,\sigma}) &= M_0(e|G),\\
n_u(e|G_{\omega,\sigma}) &= \sum_{x\in N_u(e|G)} \omega(x),\\
n_0(e|G_{\omega,\sigma}) &= \sum_{x\in N_0(e|G)} \omega(x),\\
m_u(e|G_{\omega,\sigma}) &= \sum_{f\in M_u(e|G)} \sigma(f) + \sum_{x\in N_u(e|G)} \omega(x),\\
m_0(e|G_{\omega,\sigma}) &= \sum_{f\in M_0(e|G)} \sigma(f) + \sum_{x\in N_0(e|G)} \omega(x).
\end{aligned}$$

For our main results, we introduce the definition of the *revised weighted (edge-) Szeged index* $Sz^*(G_{\omega,\sigma})$ ($Sz_e^*(G_{\omega,\sigma})$) of a vertex-edge-weighted graph $G_{\omega,\sigma}$, which was similarly mentioned in [1,4].

Definition 2.1. *Let $G_{\omega,\sigma}$ be a connected vertex-edge-weighted graph (G,ω,σ). Then we define the revised weighted (edge-)Szeged index of $G_{\omega,\sigma}$ as follows:*

$$Sz^*(G_{\omega,\sigma}) = \sum_{e=uv\in E(G)} \sigma(e)(n_u(e|G_{\omega,\sigma}) + \frac{1}{2}n_0(e|G_{\omega,\sigma}))(n_v(e|G_{\omega,\sigma}) + \frac{1}{2}n_0(e|G_{\omega,\sigma})).$$

$$Sz_e^*(G_{\omega,\sigma}) = \sum_{e=uv\in E(G)} \sigma(e)(m_u(e|G_{\omega,\sigma}) + \frac{1}{2}m_0(e|G_{\omega,\sigma}))(m_v(e|G_{\omega,\sigma}) + \frac{1}{2}m_0(e|G_{\omega,\sigma})).$$

Note that if $\omega(V) = \sigma(E) = 1$, we have $Sz^*(G_{\omega,\sigma}) = Sz^*(G)$, and if $\omega(V) = 0$ and $\sigma(E) = 1$ we have $Sz_e^*(G_{\omega,\sigma}) = Sz_e^*(G)$.

Definition 2.2. *[14] Let G be a connected graph. A partition $\mathfrak{F} = \{F_1, F_2, \cdots, F_l\}$ of $E(G)$ is* coarser *than $\mathfrak{E}$ if each edge set F_i is one or more union of sets in $\mathfrak{E}$.*

Under the statement of Definition 2.2, let C_j^i, $C_{j'}^i$ be connected components in $G_i = G - F_i$, denote by $E(C_j^i, C_{j'}^i)$ the set of edges in F_i which join a vertex from C_j^i to $C_{j'}^i$ and by $|E(C_j^i, C_{j'}^i)|$ its cardinality. We similarly define the graphs G_i^* with vertex set $V(G_i^*) = \{C_1^i, \cdots, C_{m_i}^i\}$ and the vertices C_j^i and $C_{j'}^i$ are adjacent if and only if some edge in F_i joins a vertex in C_j^i to a vertex in $C_{j'}^i$. Construct weighted graphs $G_{\omega,\sigma}^i$ with the underlying simple graph G_i^*, $\omega(C_j^i) = |V(C_j^i)|$ and $\sigma(C_j^i, C_{j'}^i) = |E(C_j^i, C_{j'}^i)|$, graphs $G_{\omega',\sigma}^i$ with the underlying simple graph G_i^*, $\omega'(C_j^i) = |E(C_j^i)|$ and $\sigma(C_j^i, C_{j'}^i) = |E(C_j^i, C_{j'}^i)|$.

We also need the following lemmas.

Lemma 2.3. *[17] Let G be a connected graph. Then G has an isometric embedding in a power of K_3 if and only if the relation θ is transitive on $E(G)$.*

Lemma 2.4. *[6]*

(1) The canonical embedding $\alpha : G \to \Box_{i=1}^k G_i^*$ is irredundant, has reducible factors and has the largest possible factors among all irredundant isometric embeddings of G.

(2) The only irredundant isometric embedding of G into a product of $dim_I(G)$ factors is the canonical embedding, where $dim_I(G)$ is the number of factors G_i^* in the canonical embedding of G.

Combining Lemma 2.4 with the proof of Lemma 2.3 in [17], we can obtain the following well-known result, which was also mentioned as a fact in [12].

Proposition 2.5. *Let G be a connected graph. If the θ relation is transitive and $(E_1, \cdots, E_k)$ are the equivalent classes, then each subgraph $G - E_i$, $i = 1, \cdots, k$, contains at most three connected components.*

3 Main Results

We shall prove several theorems and corollaries in the following.

Theorem 3.1. *Let G be a connected graph and $E_1, \cdots, E_k$ be the θ^* classes of $E(G)$. Then we have*

$$(1)\quad Sz^*(G) = \sum_{i=1}^{k} Sz^*(G^i_{\omega,\sigma}).$$

$$(2)\quad Sz^*_e(G) = \sum_{i=1}^{k} Sz^*_e(G^i_{\omega',\sigma}).$$

Proof.

(1) For each edge $e = uv \in E(G)$, there is an i such that $e \in E_i$. Note that $d_{G_i^*}(\alpha_i(x), \alpha_i(u)) - d_{G_i^*}(\alpha_i(x), \alpha_i(v))$ represents the difference of distances in graph G_i^*. Consider the relationship between $d_G(x,u) - d_G(x,v)$ and $d_{G_i^*}(\alpha_i(x), \alpha_i(u))$ $- d_{G_i^*}(\alpha_i(x), \alpha_i(v))$.

Consequently, from the canonical isometric embedding, $\alpha(u)$ and $\alpha(v)$ differ exactly on one coordinate, say the ith coordinate. So for each x and every $j \neq i$, we have $d_{G_j^*}(\alpha_j(x), \alpha_j(u)) = d_{G_j^*}(\alpha_j(x), \alpha_j(v))$. Thus we can obtain that the differences are exactly equal, i.e.,

$$\begin{aligned}
d_G(x,u) - d_G(x,v) &= d_{G^*}(\alpha(x), \alpha(u)) - d_{G^*}(\alpha(x), \alpha(v)) && (3.1)\\
&= \sum_{j=1}^{k} d_{G_j^*}(\alpha_j(x), \alpha_j(u)) - d_{G_j^*}(\alpha_j(x), \alpha_j(v)) && (3.2)\\
&= d_{G_i^*}(\alpha_i(x), \alpha_i(u)) - d_{G_i^*}(\alpha_i(x), \alpha_i(v)). && (3.3)
\end{aligned}$$

Hence for each edge $e = uv \in E(G)$, $n_u(e)$ counts the number $\sum_{C_j^i \in N_u(e|G_i^*)} |V(C_j^i)|$ and $n_0(e)$ counts the number $\sum_{C_j^i \in N_0(e|G_i^*)} |V(C_j^i)|$. Thus we conclude

$$\begin{aligned}
\left(n_u(e) + \frac{1}{2} n_0(e)\right)\left(n_v(e) + \frac{1}{2} n_0(e)\right) = &\left(\sum_{C_j^i \in N_u(e|G_i^*)} |V(C_j^i)| + \frac{1}{2} \sum_{C_j^i \in N_0(e|G_i^*)} |V(C_j^i)|\right)\\
&\left(\sum_{C_j^i \in N_v(e|G_i^*)} |V(C_j^i)| + \frac{1}{2} \sum_{C_j^i \in N_0(e|G_i^*)} |V(C_j^i)|\right).
\end{aligned}$$

Therefore $\sum_{e \in E_i} (n_u(e) + \frac{1}{2} n_0(e))(n_v(e) + \frac{1}{2} n_0(e)) = Sz^*(G^i_{\omega,\sigma})$, i.e.,

$$Sz^*(G) = \sum_{i=1}^{k} Sz^*(G^i_{\omega,\sigma}).$$

(2) Similarly, for an edge $e = uv \in E(G)$, assume $e \in E_i$. Consider each edge $f = wz \in E(G)$ other than e. Denote the unique coordinate distinguishing w and z by l.

Case 1: $l = i$.

It is obvious that $l = i$ if and only if f is an edge in G_i^*.

Suppose $d_G(f,u) - d_G(f,v) = d_G(x,u) - d_G(y,v)$, where $x, y \in \{w, z\}$. Thus $d_G(x,u) \leq d_G(y,u)$ and $d_{G_i^*}(\alpha_i(x), \alpha_i(u)) \leq d_{G_i^*}(\alpha_i(y), \alpha_i(u))$, therefore we have

$$d_{G_i^*}(\alpha_i(w)\alpha_i(z), \alpha_i(u)) = d_{G_i^*}(\alpha_i(x), \alpha_i(u)).$$

And similarly,

$$d_{G_i^*}(\alpha_i(w)\alpha_i(z), \alpha_i(v)) = d_{G_i^*}(\alpha_i(y), \alpha_i(v)).$$

Moreover,

$$\begin{aligned}
d_G(f,u) - d_G(f,v) &= d_G(x,u) - d_G(y,v) && (3.4)\\
&= d_{G^*}(\alpha(x), \alpha(u)) - d_{G^*}(\alpha(y), \alpha(v)) && (3.5)\\
&= \sum_{j=1}^{k} d_{G_j^*}(\alpha_j(x), \alpha_j(u)) - d_{G_j^*}(\alpha_j(y), \alpha_j(v)) && (3.6)\\
&= d_{G_i^*}(\alpha_i(x), \alpha_i(u)) - d_{G_i^*}(\alpha_i(y), \alpha_i(v)) && (3.7)\\
&= d_{G_i^*}(\alpha_i(w)\alpha_i(z), \alpha_i(u)) - d_{G_i^*}(\alpha_i(w)\alpha_i(z), \alpha_i(v)). && (3.8)
\end{aligned}$$

Hence we know for edges in the same equivalent class as $e = uv$, the difference of its distance from u and v equals the distance from its image between $\alpha_i(u)$ and $\alpha_i(v)$ in G_i^*.

Case 2: $l \neq i$.

Similarly, $l \neq i$ if and only if f is a vertex in G_i^*, i.e., $\alpha_i(w) = \alpha_i(z)$.

Since e and f are not in the same equivalent class, we have $d_G(u,w) + d_G(v,z) = d_G(u,z) + d_G(v,w)$. Thus if $d_G(u,w) \leq d_G(v,w)$, then $d_G(v,z) \geq d_G(u,z)$ holds. Suppose $d_G(f,u) - d_G(f,v) = d_G(x,u) - d_G(x,v)$. Then we have

$$\begin{aligned}
d_G(f,u) - d_G(f,v) &= d_G(x,u) - d_G(x,v) && (3.9)\\
&= d_{G^*}(\alpha(x), \alpha(u)) - d_{G^*}(\alpha(x), \alpha(v)) && (3.10)\\
&= \sum_{j=1}^{k} d_{G_j^*}(\alpha_j(x), \alpha_j(u)) - d_{G_j^*}(\alpha_j(x), \alpha_j(v)) && (3.11)\\
&= d_{G_i^*}(\alpha_i(x), \alpha_i(u)) - d_{G_i^*}(\alpha_i(x), \alpha_i(v)). && (3.12)
\end{aligned}$$

Hence we know for edges in the different equivalent class with $e = uv$, the difference of its distance from u and v equals the distance between its image (as a point) with $\alpha_i(u)$ and $\alpha_i(v)$ in G_i^*.

Above all, we conclude that $m_u(e) = \sum_{f\in M_u(e|G_i^*)}\sigma(f) + \sum_{x\in N_u(e|G_i^*)}\omega(x)$, $m_0(e) = \sum_{f\in M_0(e|G_i^*)}\sigma(f) + \sum_{x\in N_0(e|G_i^*)}\omega(x)$, and $\sum_{e\in E_i}(m_u(e) + \frac{1}{2}m_0(e))(m_u(e) + \frac{1}{2}m_0(e)) = Sz_e^*(G_{\omega,\sigma})$, which completes the proof. ■

From the proof of Theorem 3.1, the following corollary follows naturally, which reveals several properties of θ^*.

Corollary 3.2. *Let G be a connected graph and $E_1, \cdots, E_k$ be the θ^* classes of $E(G)$. Then for each edge $e = uv \in E_i$, $u \in C_u^i$ and $v \in C_v^i$, we have*

(1) for all vertices x in one connected component C_j^i in G_i, the values of $d_G(x,u) - d_G(x,v)$ are the same. In particular, for each x in C_u^i, $d_G(x,u) < d_G(x,v)$, and for each y in C_v^i, $d_G(y,v) < d_G(y,u)$.

(2) if $e' = u'v' \in E_i$ joins u' in C_u^i to v' in C_v^i, then $d_G(u,u') + d_G(v,v') \neq d_G(u,v') + d_G(v,u')$.

Utilizing Proposition 2.5, we can deduce Theorem 3.3, which is also a special case of Theorem 3.1(1).

Theorem 3.3. *Let G be a connected graph, θ be transitive, and $E_1, \cdots, E_k$ be the θ classes of $E(G)$. Then we have*

$$Sz^*(G) = \sum_{i=1}^{k}\sum_{C_j^i, C_{j'}^i \in V(G_i^*)} |E(C_j^i, C_{j'}^i)|(|V(C_j^i)| + \frac{1}{2}(n - |V(C_j^i)| - |V(C_{j'}^i)|))\Big(|V(C_{j'}^i)| + \frac{1}{2}(n - |V(C_j^i)| - |V(C_{j'}^i)|)\Big).$$

Proof. At first we show the following claim.

***Claim**: In each $G - E_i$ with exactly three connected components, for each $e = uv \in E_i$, there exists a connected component in which each vertex has the same distance to u as to v.*

It is clear that as long as we can prove the claim, we shall get Theorem 3.3 directly.

It suffices to prove that for each $G - E_i$ with exactly three connected components, the corresponding graph G_i^* is K_3. If it is not the case, then G_i^* has to be a P_3 and let the path be $C_1^iC_2^iC_3^i$. For each $e = uv \in E_i$ with $u \in C_1^i$ and $v \in C_2^i$, each $x \in C_2^i$, due to Corollary 3.2, we have $d_G(x,v) < d_G(x,u)$. In particular, for each $e' = u'v' \in E_i$ with $u' \in C_2^i$ and $v' \in C_3^i$, we have $d_G(u',v) < d_G(u',u)$. Since G_i^* is a P_3, then $d_G(v',u) = d_G(u',u) + 1$ and

$d_G(v',v) = d_G(u',v)+1$. Thus $d_G(u',u)+d_G(v',v) = d_G(u',v)+d_G(v',u)$, a contradiction. ■

Note: Similar to Theorem 3.3, we also have an expansion formula of the revised edge-Szeged index for the graphs mentioned above, but its has a far more complex form, so we omit it here.

In fact, for convenience when computing, we show a stronger result than Theorem 3.1.

Theorem 3.4. *Let G be a connected graph and $\mathfrak{F} = \{F_1, \cdots, F_l\}$ be a partition of E(G) coarser than $\mathfrak{E}$. Then we have*

$$(1)\quad Sz^*(G) = \sum_{i=1}^{l} Sz^*(G^i_{\omega,\sigma}).$$

$$(2)\quad Sz^*_e(G) = \sum_{i=1}^{l} Sz^*_e(G^i_{\omega',\sigma}).$$

Before proving Theorem 3.4, we show a useful lemma.

Lemma 3.5. *Let G be a connected graph and $\mathfrak{F} = \{F_1, \cdots, F_l\}$ be a partition of E(G) coarser than $\mathfrak{E}$. Define a map $\beta : V(G) \to V(G^*) = V(\Box_{i=1}^{l} G_i^*)$ to be $\beta(v) = (\beta_1(v), \ldots, \beta_l(v))$, where $\beta_i : V(G) \to V(G_i^*)$ and $v \in \beta_i(v)$. Then β is isometric.*

Proof.

To avoid confusion, denote the G_i^* corresponding with E_i by H_i^* in this proof.

It suffices to prove, without loss of generality, that when $\mathfrak{F} = \{E_1, E_2, \cdots, F_{k-1} = E_{k-1} \cup E_k\}$, the corresponding β is isometric, i.e., $d_G(u,v) = \sum_{i=1}^{k-1} d_{G_i^*}(\beta_i(u), \beta_i(v))$ for all $u, v \in V(G)$. Moreover, $d_G(u,v) = \sum_{i=1}^{k} d_{H_i^*}(\alpha_i(u), \alpha_i(v))$. Thus all we need to prove is that for all $u, v \in V(G)$, $d_{G_{k-1}^*}(\beta_{k-1}(u), \beta_{k-1}(v)) = d_{H_{k-1}^*}(\alpha_{k-1}(u), \alpha_{k-1}(v)) + d_{H_k^*}(\alpha_k(u), \alpha_k(v))$.

Considering the graphs G_{k-1}^* and $H_{k-1}^* \Box H_k^*$, each vertex $\beta_{k-1}(u)$ (a representative element) in G_{k-1}^* corresponds to a unique vertex $(\alpha_{k-1}(u), \alpha_k(u))$ (a representative element) in $H_{k-1}^* \Box H_k^*$ and the map is injective. Moreover, if vertices $(\alpha_{k-1}(u), \alpha_k(u))$ and $(\alpha_{k-1}(v), \alpha_k(v))$ are adjacent in $H_{k-1}^* \Box H_k^*$, then vertices $\beta_{k-1}(u)$ and $\beta_{k-1}(v)$ are adjacent in G_{k-1}^*. Thus G_{k-1}^* is an induced subgraph of $H_{k-1}^* \Box H_k^*$, and $u, v \in V(G)$, $d_{G_{k-1}^*}(\beta_{k-1}(u), \beta_{k-1}(v)) \geq d_{H_{k-1}^*}(\alpha_{k-1}(u), \alpha_{k-1}(v)) + d_{H_k^*}(\alpha_k(u), \alpha_k(v))$.

On the other hand, for $u, v \in V(G)$ and each shortest (u,v)-path P in G, $|P \cap E_{k-1}| = d_{H_{k-1}^*}(\alpha_{k-1}(u), \alpha_{k-1}(v))$ and $|P \cap E_k| = d_{H_k^*}(\alpha_k(u), \alpha_k(v))$. Moreover, $P \cap E_{k-1}, P \cap$

$E_k \subseteq E(H^*_{k-1})$. Since $H^*_{k-1}[(P \cap E_{k-1}) \cup (P \cap E_k)]$ induces a path between $\beta_{k-1}(u)$ and $\beta_{k-1}(v)$, we have for all $u, v \in V(G)$, $d_{G^*_{k-1}}(\beta_{k-1}(u), \beta_{k-1}(v)) \leq d_{H^*_{k-1}}(\alpha_{k-1}(u), \alpha_{k-1}(v)) + d_{H^*_k}(\alpha_k(u), \alpha_k(v))$, which completes the proof. ■

Proof of Theorem 3.4.

Note that $G^i_{\omega,\sigma}$ and $G^i_{\omega',\sigma}$ have been defined in Section 2 with respect to $\mathfrak{F}$. Since β is an isometric embedding by Lemma 3.5, the proof is almost the same as the one in Theorem 3.1 and we omit it here. ■

4 Examples

In this section, we will give two examples to show how to use our formula to calculate the revised (edge-)Szeged indices. Denote by $Sz^*(e)$ the number $(n_u(e) + \frac{1}{2}n_0(e))(n_v(e) + \frac{1}{2}n_0(e))$ and by $Sz^*_e(f)$ the number $(m_u(f) + \frac{1}{2}m_0(f))(m_v(f) + \frac{1}{2}m_0(f))$.

4.1 Example 1

As Example 1 we calculate the revised Szeged index of the molecular graph of porphin $C_{20}H_{14}N_4$ (omitting trivial branches). The molecular graph is shown in Figure 1.

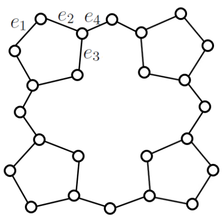

Figure 1. G and its edge labels.

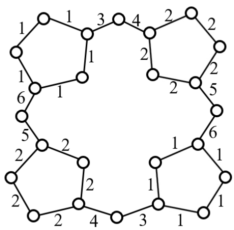

Figure 2. G and its six equivalent classes.

Since the subtle symmetry of G, the calculation of $Sz^*(G)$ can be reduced to $Sz^*(G) = 4Sz^*(e_1) + 8Sz^*(e_2) + 8Sz^*(e_3) + 8Sz^*(e_4)$.

We show the distance relationship in Figures 3, 4, 5, 6 where the vertex labelling u, v or w is nearer to u, v or the same close to u and v, respectively. Thus

$Sz^*(G) = 4 \times (11 + \frac{1}{2} \times 2)(11 + \frac{1}{2} \times 2) + 8 \times (2 + \frac{1}{2} \times 9)(13 + \frac{1}{2} \times 9) + 8 \times (10 + \frac{1}{2} \times 2)(12 + \frac{1}{2} \times 2) + 8 \times 12 \times 12 = 3782$.

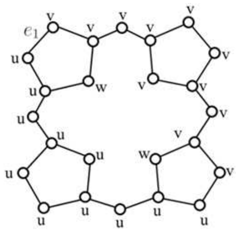

Figure 3. the distance relationships according to edge e_1.

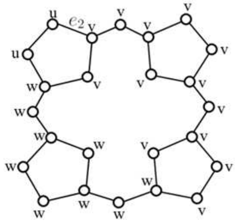

Figure 4. the distance relationships according to edge e_2.

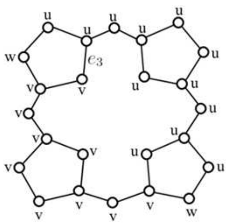

Figure 5. the distance relationships according to edge e_3.

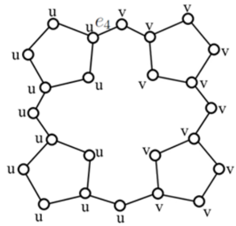

Figure 6. the distance relationships according to edge e_4.

On the other hand, we calculate the value by Theorem 3.1 through the graphs $G^i_{\omega,\sigma}$, $i = 1, \cdots, 6$. We only show $G - E_1, G - E_3, G^1_{\omega,\sigma}, G^3_{\omega,\sigma}$ in Figures 7, 8 and omit the isomorphic ones. Utilizing Theorem 3.1, we reduce the calculation to

$$Sz^*(G) = \sum_{i=1}^{6} Sz^*(G^i_{\omega,\sigma}) \tag{4.1}$$

$$= 2 \times (4 \times (13 + \frac{1}{2} \times 9)(2 + \frac{1}{2} \times 9) + 2 \times (11 + \frac{1}{2} \times 2)(11 + \frac{1}{2} \times 2)+$$

$$4 \times (12 + \frac{1}{2} \times 2)(10 + \frac{1}{2} \times 2)) + 4 \times (2 \times 12 \times 12) \tag{4.2}$$

$$= 3782. \tag{4.3}$$

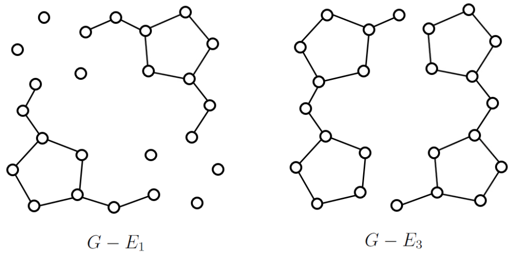

Figure 7. $G - E_1 \cong G - E_2$ and $G - E_3 \cong G - E_i, i = 4, 5, 6$.

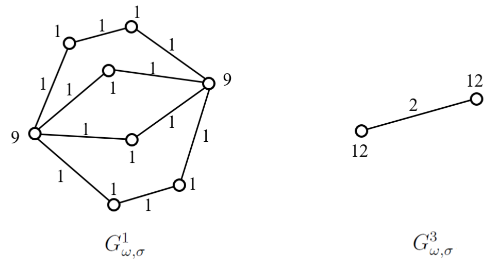

Figure 8. $G^1_{\omega,\sigma} \cong G^2_{\omega,\sigma}$ and $G^3_{\omega,\sigma} \cong G^i_{\omega,\sigma}, i = 4, 5, 6$.

4.2 Example 2

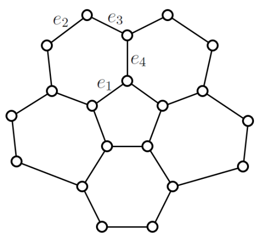

Figure 9. G and its edge labels.

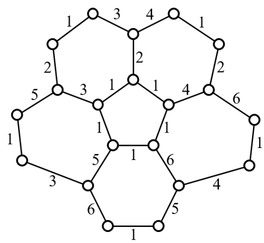

Figure 10. G and its six equivalent classes.

Now we look at another example, the graph G (part of the Carbon 60) shown in Figure 9. We can reduce the calculation of $Sz_e^*(G)$ to $Sz_e^*(G) = 5Sz_e^*(e_1) + 5Sz_e^*(e_2) + 10Sz_e^*(e_3) + 5Sz_e^*(e_4)$.

The distance relationship is shown in Figures 11, 12, 13, 14. Consequently we have

$Sz_e^*(G) = 5 \times (10 + \frac{5}{2}) \times (10 + \frac{5}{2}) + 5 \times (10 + \frac{5}{2}) \times (10 + \frac{5}{2}) + 10 \times (4 + \frac{3}{2}) \times (18 + \frac{3}{2}) + 5 \times (4 + \frac{3}{2})(18 + \frac{3}{2}) = 2586.25$.

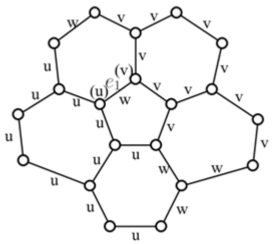

Figure 11. the distance relationships according to edge e_1.

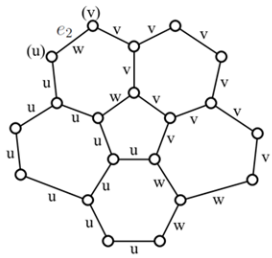

Figure 12. the distance relationships according to edge e_2.

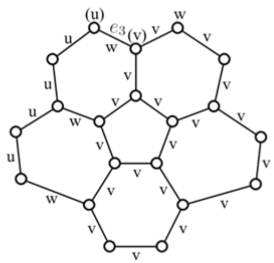

Figure 13. the distance relationships according to edge e_3.

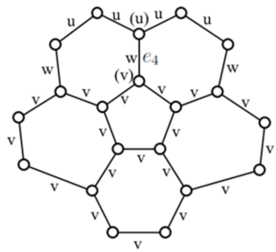

Figure 14. the distance relationships according to edge e_4.

Next, we calculate the value by Theorem 3.1 through the graphs $G^i_{\omega',\sigma}, i = 1, \cdots, 6$. We only show $G - E_1, G - E_2, G^1_{\omega',\sigma}, G^2_{\omega',\sigma}$ in Figures 15, 16 as representatives.

$$Sz_e^*(G) = \sum_{i=1}^{6} Sz_e^*(G^i_{\omega',\sigma}) \tag{4.4}$$

$$= 5 \times 2 \times ((2+2+3+3) + \frac{1}{2}(2+3))((2+2+3+3) + \frac{1}{2}(2+3))+$$

$$5 \times 3 \times (18 + \frac{3}{2})(4 + \frac{3}{2}) \tag{4.5}$$

$$= 2586.25. \tag{4.6}$$

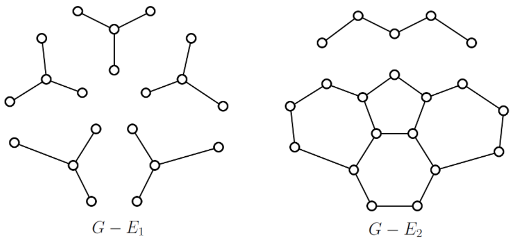

Figure 15. $G - E_2 \cong G - E_i, i = 3, 4, 5, 6.$

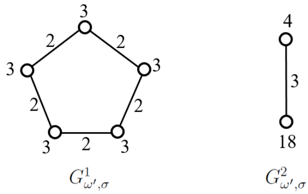

Figure 16. $G^2_{\omega',\sigma} \cong G^i_{\omega',\sigma}, i = 3, 4, 5, 6.$

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