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On the Randić Index of Polymeric Networks Modelled by Generalized Sierpiński Graphs

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Abstract

The Randić index R of a simple graph G is defined as

$$R(G) = \sum_{v_i \sim v_j} \frac{1}{\sqrt{\delta_i \delta_j}}\,,$$

where δ_i denotes the degree of the vertex v_i. In this paper we obtain closed formulae for the Randić index of Sierpiński-type polymeric networks.

1 Introduction

Over the past three decades, polymer networks has emerged as a coherent subject area. It is well-known that, in comparison with those linear polymers, the properties of polymer networks depend to a much larger extent on methods and condition of preparation, *i.e.,* properties depend not only on the chemical structure of the individual polymer chains, but on how those chains are joined together to form a network [26]. While the basic works on polymer modelling started from linear polymeric systems, in recent years the attention has focused more and more on complex underlying geometries including fractals generalized networks. In this article we consider a model of polymer networks based on generalized Sierpiński graphs.

To begin with, we need some notation and terminology. Let $G = (V, E)$ be a non-empty graph of order n and vertex set $V = \{1, 2, ..., n\}$. We denote by $\{1, 2, ..., n\}^t$ the set of words of size t on alphabet $\{1, 2, ..., n\}$. The letters of a word u of length t are denoted by $u_1u_2...u_t$. The concatenation of two words u and v is denoted by uv. Klavžar and Milutinović introduced in [12] the graph $S(K_n, t)$ whose vertex set is $\{1, 2, ..., n\}^t$, where $\{u, v\}$ is an edge if and only if there exists $i \in \{1, ..., t\}$ such that:

(i) $u_j = v_j$, if $j < i$;

(ii) $u_i \neq v_i$;

(iii) $u_j = v_i$ and $v_j = u_i$ if $j > i$.

When $n = 3$, those graphs are exactly Tower of Hanoi graphs. Later, those graphs have been called Sierpiński graphs in [13] and they were studied by now from numerous points of view. The reader is invited to read, for instance, the following recent papers [5,7,8,13–15] and references therein.

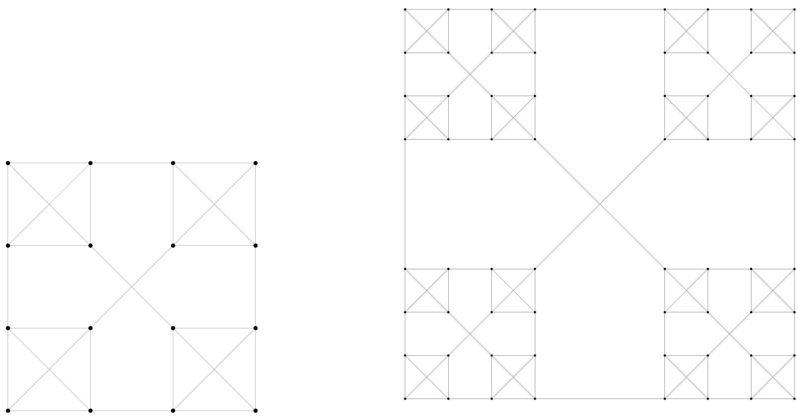

Figure 1: Two Sierpiński graphs: $S(K_4, 2)$ and $S(K_4, 3)$.

Figure 1 shows the Sierpiński graphs $S(K_4, 2)$ and $S(K_4, 3)$. This construction was generalized in [4] for any graph G, by defining the *generalized Sierpiński graph*, $S(G, t)$, as the graph with vertex set $\{1, 2, ..., n\}^t$ and edge set defined as follows. $\{u, v\}$ is an edge if and only if there exists $i \in \{1, ..., t\}$ such that:

(i) $u_j = v_j$, if $j < i$;

(ii) $u_i \neq v_i$ and $\{u_i, v_i\} \in E$;

(iii) $u_j = v_i$ and $v_j = u_i$ if $j > i$.

Notice that if $\{u, v\}$ is an edge of $S(G, t)$, there is an edge $\{x, y\}$ of G and a word w such that $u = wxyy...y$ and $v = wyxx...x$. In general, $S(G, t)$ can be constructed recursively from G with the following process: $S(G, 1) = G$ and, for $t \geq 2$, we copy n times $S(G, t-1)$ and add the letter x at the beginning of each label of the vertices belonging to the copy of $S(G, t-1)$ corresponding to x. Then for every edge $\{x, y\}$ of G, add an edge between vertex $xyy...y$ and vertex $yxx...x$. See, for instance, Figure 2. Vertices of the form $xx...x$ are called *extreme vertices*. Notice that for any graph G of order n and any integer $t \geq 2$, $S(G, t)$ has n extreme vertices and, if x has degree $d(x)$ in G, then the extreme vertex $xx...x$ of $S(G, t)$ also has degree $d(x)$. Moreover, the degrees of two vertices $yxx...x$ and $xyy...y$, which connect two copies of $S(G, t-1)$, are equal to $d(x) + 1$ and $d(y) + 1$, respectively.

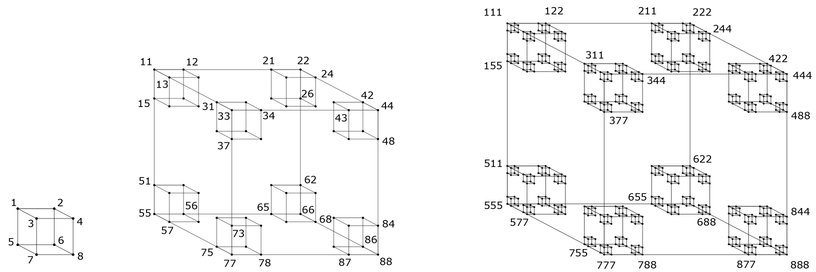

Figure 2: The 3-cube graph Q_3 and the Sierpiński graphs $S(Q_3, 2)$ and $S(Q_3, 3)$.

We denote by P_r the path graph of order r. Notice that for $G = K_2$ we obtain $S(K_2, 2) = P_4$ and, in general, $S(K_2, t) = P_{2^t}$, which is the simplest possible polymer model presented by the ideal chain. Also, the graphs $S(K_n, t)$ were used in [1, 10, 11] to analyse the scaling behaviour of experimentally accessible dynamical relaxation forms for polymers modelled through finite Sierpiński-type graphs, which we denote here by $P(K_n, t)$. Using the approach introduced in [10, 11] to construct $P(K_n, t)$, now we define the polymeric Sierpiński graphs $P(G, t) = (V, E)$, where G is a connected graph of order n and t is a positive integer. For $i \in \{1, ..., t\}$ we define the sets $A_i = \{a_{i_1}, ..., a_{i_{n^{i-1}}}\}$ and we denote $S(G, i) = (V_i, E_i)$ and $V_i = \{v_{i_1}, ..., v_{i_{n^i}}\}$. Then, the vertex set of $P(G, t)$ is

$$V = \bigcup_{i=1}^{t} (A_i \cup V_i)$$

and the edge set of $P(G, t)$ is

$$E = \left(\bigcup_{i=1}^{n} (E_i \cup B_i) \right) \cup \left(\bigcup_{i=1}^{t-1} C_i \right),$$

where $C_i = \{\{v_{i_j}, a_{i+1_j}\} : j = 1, ..., n^i\}$, $B_i = \bigcup_{j=1}^{n^{i-1}} W_j$, and W_j is formed by the edges obtained by connecting a_{i_j} to every vertex belonging to the j-th copy of G in $S(G,i)$. In other words, we construct $P(G,t)$ as follows: The iterative construction starts from one vertex, a_{1_1}, and one copy of $G = S(G,1)$. So, we obtain $P(G,1)$ by connecting a_{1_1} to every vertex of $S(G,1)$. To obtain $P(G,2)$ we take $P(G,1)$, A_2 and $S(G,2)$. Then we connect each element $a_{2_j} \in A_2$ to $v_{1_j} \in V_1$ and we also connect a_{2_j} to every vertex in the j-th copy of G in $S(G,2)$. Analogously, for the construction of $P(G,t)$ we take $P(G,t-1)$, A_t and $S(G,t)$. Then, we connect each element $a_{t_j} \in A_t$ to $v_{t-1_j} \in V_{t-1}$ and we also connect a_{t_j} to every vertex in the j-th copy of G in $S(G,t)$. Notice that $P(K_3,2) = S(K_4,2)$, $S(K_3,2) = P(K_2,2)$, while for $t \geq 3, P(K_n,t) \neq S(K_{n+1},t)$.

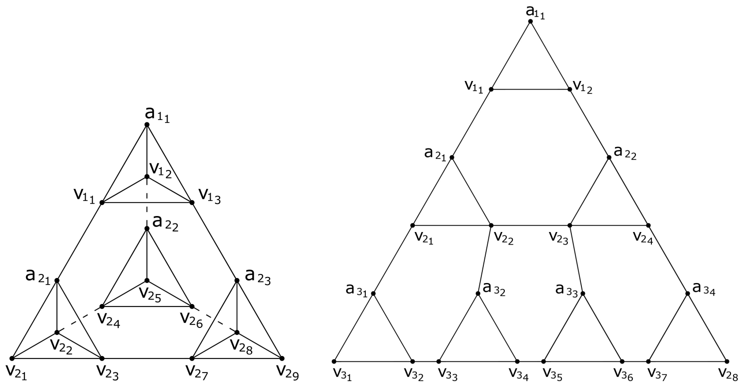

Figure 3: Two polymeric Sierpiński graphs: $P(K_3,2) = S(K_4,2)$ and $P(K_2,3)$.

Around the middle of the last century theoretical chemists proposed the use of topological indices to obtain information on the dependence of various properties of organic substances on molecular structure. In this sense, a large number of various topological indices was proposed and considered in the chemical literature [27]. We highlight the article [2] where Camarda and Maranas addressed the design of polymers with optimal levels of macroscopic properties through the use of topological indices. Specifically, in the above mentioned article two zeroth-order and two first-order connectivity indices were employed for the first time as descriptors in structure-property correlations in an optimization study. Based on these descriptors, a set of new correlations for heat capacity, cohesive energy, glass transition temperature, refractive index, and dielectric constant were proposed.

The molecular structure-descriptor, introduced in 1975 by Milan Randić in [22], is defined as

$$R(G) = \sum_{v_i v_j \in E} \frac{1}{\sqrt{d(v_i)d(v_j)}},$$

where $d(v_i)$ represents the degree of the vertex v_i in G. Nowadays, $R(G)$ is referred to as the Randić index of $G = (V, E)$. This graph topological index, sometimes referred to as *connectivity index*, has been successfully related to a variety of physical, chemical, and pharmacological properties of organic molecules and became one of the most popular molecular-structure descriptors [23]. After the publication of the first paper [22], mathematical properties and generalizations of $R(G)$ were extensively studied, for instance, see [3, 6, 9, 16–20, 24, 25, 29] and the references cited therein.

Some topological indices have been studied also for the case of polymeric networks. For instance, we cite the article [28], where the authors gave the explicitly formula of the k-connectivity index of an infinite class of dendrimer nanostars. In this article we obtain closed formulae for the Randić index of Sierpiński-type polymeric networks. In particular, we study the Randić index of $S(G, t)$ and $P(G, t)$, where G is a complete graph, a triangle free δ-regular graph and a bipartite (δ_1, δ_2)-semiregular graph.

2 Computing the Randić index of $S(G, t)$

Theorem 1. *For any integers $t, n \geq 2$, $R(S(K_n, t)) = \sqrt{n(n-1)} + \frac{n^t - 2n + 1}{2}$.*

Proof. Since $S(K_n, t)$ has n extreme vertices of degree $n-1$ and $n^t - n$ non-extreme vertices of degree n, the size of $S(K_n, t)$ is $m = \frac{n(n-1) + (n^t - n)n}{2} = \frac{n^{t+1} - n}{2}$. Now, $S(K_n, t)$ has no edges formed by extreme vertices and the number of edges containing one extreme vertex is equal to $n(n-1)$, so the number of edges non-containing extreme vertices is $\frac{n^{t+1}-n}{2} - n(n-1) = \frac{n^{t+1}-2n^2+n}{2}$. Therefore,

$$R(S(K_n, t)) = \frac{n(n-1)}{\sqrt{n(n-1)}} + \frac{n^{t+1} - 2n^2 + n}{2n} = \sqrt{n(n-1)} + \frac{n^t - 2n + 1}{2}. \qquad \blacksquare$$

From now on, given a graph H, the number of edges whose endpoints have degrees δ and δ' will be denoted by $f_H(\delta, \delta')$.

Lemma 2. *For any triangle free δ-regular graph G of order n and any integer $t \geq 2$,*

(i) $f_{S(G,t)}(\delta, \delta) = \frac{n^{t-1}\delta}{2}(n - 2\delta)$.

(ii) $f_{S(G,t)}(\delta, \delta + 1) = \left(n^{t-1} + \frac{n^{t-1} - n}{1 - n}\right)\delta^2$.

(iii) $f_{S(G,t)}(\delta+1,\delta+1) = \frac{n\delta}{2}\left(\frac{1-n^{t-1}}{1-n}\right) + n\delta^2\left(\frac{1-n^{t-2}}{1-n}\right).$

Proof. Notice that $S(G,t)$ is a semiregular graph of degrees δ and $\delta+1$.

(i) The set of vertices of degree $\delta+1$ in $S(G,2)$ is formed by the neighbours of the extreme vertices of $S(G,2)$ and, since G is a triangle free graph, each copy of G in $S(G,2)$ has $\frac{n\delta}{2}-\delta^2$ edges whose endpoints have degree δ in $S(G,2)$. Hence, $f_{S(G,2)}(\delta,\delta) = n\left(\frac{n\delta}{2}-\delta^2\right) = \frac{n\delta}{2}(n-2\delta)$.

For $t \geq 3$, any edge of $S(G,t)$ connecting two copies of $S(G,t-1)$ is formed by vertices of degree $\delta+1$ whose neighbours have degree $\delta+1$ and, as a consequence, we have that $f_{S(G,t)}(\delta,\delta) = nf_{S(G,t-1)}(\delta,\delta)$. Therefore, for any $t \geq 2$, $f_{S(G,t)}(\delta,\delta) = \dfrac{n^{t-1}\delta}{2}(n-2\delta)$.

(ii) Any vertex of degree $\delta+1$ in $S(G,2)$ is a neighbour of an extreme vertex and, since G is a triangle free graph, each copy of G contains δ^2 edges whose endpoints have degree δ and $\delta+1$ in $S(G,2)$. Hence, $f_{S(G,2)}(\delta,\delta+1) = n\delta^2$.

Let $t \geq 3$ and let S_i denote the i-th copy of $S(G,t-1)$ in $S(G,t)$. Notice that there are δ extreme vertices of S_i, of degree $\delta+1$ in $S(G,t)$, having δ neighbours in S_i and one neighbour in S_j, for some $j \neq i$. Thus, as G is a triangle free graph, there are δ^2 edges in S_i whose endpoints have degree $\delta+1$ in $S(G,t)$ and degree δ and $\delta+1$, respectively, in S_i. Hence, $f_{S(G,t)}(\delta,\delta+1) = n\left(f_{S(G,t-1)}(\delta,\delta+1)-\delta^2\right)$. Therefore, for any $t \geq 2$, $f_{S(G,t)}(\delta,\delta+1) = \left(n^{t-1}-n^{t-2}-\cdots-n\right)\delta^2 = \left(n^{t-1}+\dfrac{n^{t-1}-n}{1-n}\right)\delta^2$.

(iii) There are $\frac{n\delta}{2}$ edges $\{x,y\}$ in $S(G,2)$ whose endpoints have degree $d(x)=d(y)=\delta+1$. Now, for $t \geq 3$, there are $\frac{n\delta}{2}$ edges in $S(G,t)$, connecting different copies of $S(G,t-1)$, whose endpoints are extreme vertices in $S(G,t-1)$. All the neighbours of these extreme vertices in $S(G,t-1)$ have degree $\delta+1$ and, since G is a triangle free graph,

$$f_{S(G,t)}(\delta+1,\delta+1) = \frac{n\delta}{2} + n\left(f_{S(G,t-1)}(\delta+1,\delta+1)+\delta^2\right).$$

Hence, for any $t \geq 2$,

$$\begin{aligned} f_{S(G,t)}(\delta+1,\delta+1) &= \frac{n\delta}{2}\left(1+n+n^2+\cdots+n^{t-2}\right) + n\delta^2\left(n^{t-3}+n^{t-2}+\cdots+1\right) \\ &= \frac{n\delta}{2}\left(\frac{1-n^{t-1}}{1-n}\right) + n\delta^2\left(\frac{1-n^{t-2}}{1-n}\right). \end{aligned}$$

■

Theorem 3. *For any triangle free δ-regular graph G of order n and any integer $t \geq 2$,*

$$R(S(G,t)) = \frac{n^{t-1}}{2}(n-2\delta) + \left(n^{t-1} + \frac{n^{t-1}-n}{1-n}\right)\frac{\delta^2}{\sqrt{\delta(\delta+1)}} + \frac{n\delta}{2(\delta+1)}\left(\frac{1-n^{t-1}}{1-n}\right) + \frac{n\delta^2}{\delta+1}\left(\frac{1-n^{t-2}}{1-n}\right).$$

Proof. Since $S(G,t)$ is a semiregular graph of degrees δ and $\delta+1$,

$$R(S(G,t)) = \frac{f_{S(G,t)}(\delta,\delta)}{\delta} + \frac{f_{S(G,t)}(\delta,\delta+1)}{\sqrt{\delta(\delta+1)}} + \frac{f_{S(G,t)}(\delta+1,\delta+1)}{\delta+1}.$$

Therefore, by Lemma 2 the result immediately follows. ■

Lemma 4. *Let $G = (U_1 \cup U_2, E)$ be a bipartite (δ_1, δ_2)-semiregular graph of order $n = n_1 + n_2$, where $|U_1| = n_1$, $|U_2| = n_2$ and $\delta_1 \neq \delta_2$. Then for any integer $t \geq 2$,*

(i) $f_{S(G,t)}(\delta_1, \delta_2) = \delta_1 n^{t-1}(n_1 - \delta_2)$.

(ii) $f_{S(G,t)}(\delta_1+1, \delta_2) = \delta_1\delta_2\left(n_2 n^{t-2} - \dfrac{n_1\left(n^{t-2}-1\right)}{n-1}\right)$.

(iii) $f_{S(G,t)}(\delta_1, \delta_2+1) = \delta_1\delta_2\left(n_1 n^{t-2} - \dfrac{n_2\left(n^{t-2}-1\right)}{n-1}\right)$.

(iv) $f_{S(G,t)}(\delta_1+1, \delta_2+1) = \dfrac{n_1\delta_1\left(n^{t-1}-1\right) + n\delta_1\delta_2\left(n^{t-2}-1\right)}{n-1}$.

Proof. We have four different possibilities for the degree of any vertex in $S(G,t)$, namely δ_1, δ_2, δ_1+1 and δ_2+1. Notice that if the degree of a vertex of $S(G,t)$ belongs to $\{\delta_1, \delta_1+1\}$, then the degree of its neighbours belongs to $\{\delta_2, \delta_2+1\}$ and, by symmetry, if the degree of a vertex of $S(G,t)$ belongs to $\{\delta_2, \delta_2+1\}$, then the degree of its neighbours belongs to $\{\delta_1, \delta_1+1\}$.

(i) For any copy of G in $S(G,2)$ there are $\delta_1\delta_2$ edges having exactly one endpoint which is neighbour of an extreme vertex, the remaining edges have endpoints of degree δ_1 and δ_2 in $S(G,2)$. Moreover, any edge $\{x,y\}$ of $S(G,t)$ connecting two copies of $S(G,t-1)$ is formed by vertices of degree $d(x) = \delta_1+1$ and $d(y) = \delta_2+1$ whose neighbours have degree δ_2+1 and δ_1+1, respectively. Hence, $f_{S(G,2)}(\delta_1,\delta_2) = n(n_1\delta_1 - \delta_1\delta_2)$ and for $t \geq 3$, $f_{S(G,t)}(\delta_1,\delta_2) = nf_{S(G,t-1)}(\delta_1,\delta_2)$. Therefore, for any $t \geq 2$,

$$f_{S(G,t)}(\delta_1,\delta_2) = \delta_1 n^{t-1}(n_1 - \delta_2).$$

(ii) If $\{x, y\}$ is an edge of $S(G,2)$ such that $d(x) = \delta_1 + 1$ and $d(y) = \delta_2$, then x is neighbour of an extreme vertex of $S(G,2)$ and, as a consequence, $f_{S(G,2)}(\delta_1+1, \delta_2) = n_2\delta_1\delta_2$.

For $t \geq 3$, we denote by S_i the i-th copy of $S(G, t-1)$ in $S(G,t)$. We assume, without loss of generality, that the i-th vertex of G belongs to U_1. In this case there are δ_1 extreme vertices of S_i having δ_2+1 neighbours in $S(G,t)$, δ_2 neighbours in S_i and one neighbour in S_j, for some $j \neq i$. Thus, there are $\delta_1\delta_2$ edges in S_i whose endpoints have degree δ_2+1 and δ_1+1 in $S(G,t)$ and degree δ_2 and δ_1+1, respectively, in S_i. Hence, the contribution of S_i to $f_{S(G,t)}(\delta_1+1, \delta_2)$ is equal to $f_{S(G,t-1)}(\delta_1+1, \delta_2) - \delta_1\delta_2$. On the other hand, if the i-th vertex of G belongs to U_2, then the contribution of S_i to $f_{S(G,t)}(\delta_1+1, \delta_2)$ is equal to $f_{S(G,t-1)}(\delta_1+1, \delta_2)$. Then we have

$$f_{S(G,t)}(\delta_1+1, \delta_2) = n f_{S(G,t-1)}(\delta_1+1, \delta_2) - n_1\delta_1\delta_2.$$

Therefore, for any $t \geq 2$,

$$\begin{aligned} f_{S(G,t)}(\delta_1+1, \delta_2) &= n^{t-2}n_2\delta_1\delta_2 - n_1\delta_1\delta_2\left(n^{t-3} + n^{t-2} + \cdots + 1\right) \\ &= \delta_1\delta_2\left(n_2n^{t-2} - \frac{n_1\left(n^{t-2}-1\right)}{n-1}\right). \end{aligned}$$

(iii) This case is analogous to the previous one.

(iv) There are $n_1\delta_1 = n_2\delta_2$ edges in $S(G,2)$ whose endpoints have degree δ_1+1 and δ_2+1. Now, for $t \geq 3$, there are $n_1\delta_1 = n_2\delta_2$ edges in $S(G,t)$, connecting different copies of $S(G,t-1)$, whose endpoints are extreme vertices in $S(G,t-1)$. Since all the neighbours of these extreme vertices of degree δ_1 (Resp. δ_2) in $S(G,t-1)$ have degree δ_2+1 (Resp. δ_1+1),

$$f_{S(G,t)}(\delta_1+1, \delta_2+1) = n_1\delta_1 + n\left(f_{S(G,t-1)}(\delta_1+1, \delta_2+1) + \delta_1\delta_2\right).$$

Hence, for any $t \geq 2$,

$$\begin{aligned} f_{S(G,t)}(\delta_1+1, \delta_2+1) &= n_1\delta_1\sum_{l=0}^{t-2} n^l + n\delta_1\delta_2\sum_{l=0}^{t-3} n^l \\ &= \frac{n_1\delta_1\left(n^{t-1}-1\right)}{n-1} + \frac{n\delta_1\delta_2\left(n^{t-2}-1\right)}{n-1}. \end{aligned}$$

■

Theorem 5. *Let $G = (U_1 \cup U_2, E)$ be a bipartite (δ_1, δ_2)-semiregular graph of order $n = n_1 + n_2$, where $|U_1| = n_1$ and $|U_2| = n_2$. Then for any integer $t \geq 2$,*

$$\begin{aligned} R(S(G,t)) &= \frac{\delta_1 n^{t-1}(n_1 - \delta_2)}{\sqrt{\delta_1\delta_2}} + \frac{\delta_1\delta_2}{\sqrt{(\delta_1+1)\delta_2}}\left(n_2 n^{t-2} - \frac{n_1\left(n^{t-2}-1\right)}{n-1}\right) \\ &+ \frac{\delta_1\delta_2}{\sqrt{\delta_1(\delta_2+1)}}\left(n_1 n^{t-2} - \frac{n_2\left(n^{t-2}-1\right)}{n-1}\right) + \frac{n_1\delta_1\left(n^{t-1}-1\right) + n\delta_1\delta_2\left(n^{t-2}-1\right)}{(n-1)\sqrt{(\delta_1+1)(\delta_2+1)}}. \end{aligned}$$

Proof. If $\delta_1 = \delta_2$, then we are done by Theorem 3. If $\delta_1 \neq \delta_2$, then we have four possibilities for the degree of any vertex in $S(G,t)$, namely δ_1, δ_2, δ_1+1 and δ_2+1. Hence,

$$R(S(G,t)) = \frac{f_{S(G,t)}(\delta_1,\delta_2)}{\sqrt{\delta_1\delta_2}} + \frac{f_{S(G,t)}(\delta_1+1,\delta_2)}{\sqrt{(\delta_1+1)\delta_2}} + \frac{f_{S(G,t)}(\delta_1,\delta_2+1)}{\sqrt{\delta_1(\delta_2+1)}} + \frac{f_{S(G,t)}(\delta_1+1,\delta_2+1)}{\sqrt{(\delta_1+1)(\delta_2+1)}}.$$

Therefore, by Lemma 4 the result immediately follows. ■

Chemical trees are trees that have no vertex with degree greater than 4. For instance, Figure 4 shows the chemical tree $S(K_{1,3}, 2)$. Notice that for any $t \geq 2$, the Sierpiński graph $S(K_{1,3}, t)$, is a chemical tree.

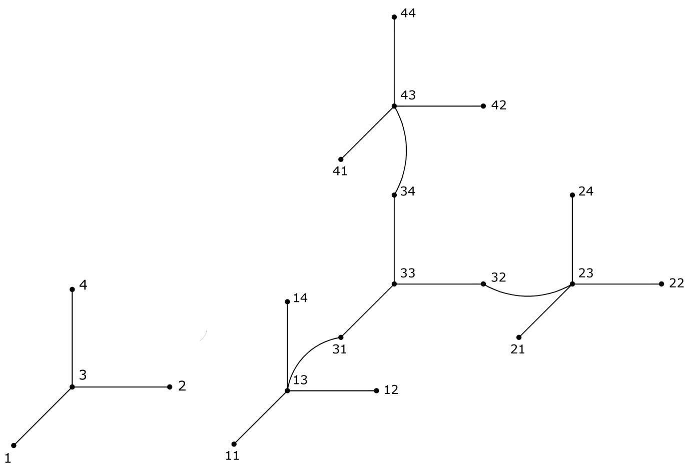

Figure 4: The graph $K_{1,3}$ and the Sierpiński graph $S(K_{1,3}, 2)$.

As a particular case of Theorem 5 we obtain the following corollary.

Corollary 6. *For any integers $r, t \geq 2$,*

$$R(S(K_{1,r},t)) = \frac{(r+1)^{t-1}(r-1)+1}{\sqrt{r+1}} + \sqrt{\frac{r}{2}} + \frac{2(r+1)^{t-1}-r-2}{\sqrt{2(r+1)}}.$$

3 Computing the Randić index of $P(G, t)$

Since $P(K_n, 1) \cong K_{n+1}$, we have $R(P(K_n, 1)) = \dfrac{n+1}{2}$. For $t \geq 2$ we have the following result.

Theorem 7. *For any integers $n, t \geq 2$,*

$$R(P(K_n, t)) = \sum_{l=1}^{5} \alpha_l,$$

where $\alpha_1 = \sqrt{n(n+1)}$, $\alpha_2 = \frac{n(n^t+2n^{t-1}-n+4t-8)}{2(n+1)}$, $\alpha_3 = \frac{n^{t+1}-n^3+(t-2)(n-1)(n-2n^2)}{2(n+2)(n-1)}$, $\alpha_4 = \frac{2n^t-n^2-n}{(n-1)\sqrt{(n+1)(n+2)}}$ *and* $\alpha_5 = \frac{(t-2)(n^2-2n)-n(t-1)}{\sqrt{(n+1)(n+2)}}$.

Proof. Let $d(x)$ be the degree of x in $P(G, t)$. We differentiate the following cases for the edges $\{x, y\}$ of $P(G, t)$.

(1) $x = a_{1_1}$ and $y \in V_1$. In this case, there are n edges $\{x, y\}$ with $d(x) = n$ and $d(y) = n + 1$. Then the contribution of these edges to the Randić index is

$$\zeta_1 = \sqrt{\frac{n}{n+1}}\ .$$

(2) $x, y \in V_1$. In this case, there are $\frac{n(n-1)}{2}$ edges $\{x, y\}$ with $d(x) = d(y) = n + 1$. So, the contribution of these edges to the Randić index is

$$\zeta_2 = \frac{n(n-1)}{2(n+1)}\ .$$

(3) $x \in A_i$ and $y \in V_i$, for $2 \leq i \leq t - 1$. There are n edges $\{x, y\}$ where y is an extreme vertex of $S(K_n, i)$ and for these vertices we have $d(x) = d(y) = n + 1$. Moreover, there are $n^i - n$ edges $\{x, y\}$ where y is not an extreme vertex of $S(K_n, i)$ and in this case we have $d(x) = n+1$ and $d(y) = n+2$. Thus, the contribution of these edges to the Randić index is

$$\begin{aligned}\zeta_3 &= \sum_{i=2}^{t-1}\left(\frac{n}{n+1} + \frac{n^i - n}{\sqrt{(n+1)(n+2)}}\right)\\ &= \frac{(t-2)n}{n+1} + \frac{n^2(n^{t-2}-1)}{(n-1)\sqrt{(n+1)(n+2)}} - \frac{(t-2)n}{\sqrt{(n+1)(n+2)}}.\end{aligned}$$

(4) $x, y \in V_i$, for $2 \leq i \leq t - 1$. There are $n(n - 1)$ edges $\{x, y\}$ where x is an extreme vertex of $S(K_n, i)$, and for these vertices we have $d(x) = n + 1$ and $d(y) = n + 2$. Also, we know that the size of $S(K_n, i)$ is $\frac{n^{i+1}-n}{2}$, so there are $\frac{n^{i+1}-n}{2} - n(n-1)$ edges

$\{x, y\}$ where neither x nor y are extreme vertices of $S(K_n, i)$ and for these vertices we have $d(x) = d(y) = n + 2$. Hence, in this case the contribution of these edges to the Randić index is

$$\zeta_4 = \sum_{i=2}^{t-1} \left(\frac{n(n-1)}{\sqrt{(n+1)(n+2)}} + \frac{n^{i+1} + n - 2n^2}{2(n+2)} \right)$$
$$= \frac{(t-2)n(n-1)}{\sqrt{(n+1)(n+2)}} + \frac{n^3(n^{t-2} - 1)}{2(n+2)(n-1)} + \frac{(t-2)(n-2n^2)}{2(n+2)}.$$

(5) $x \in V_i$ and $y \in A_{i+1}$, for $1 \le i \le t - 1$. There are n edges $\{x, y\}$ where x is an extreme vertex of $S(K_n, i)$ and for these vertices $d(x) = d(y) = n + 1$. Moreover, for the remaining $n^i - n$ edges we have $d(x) = n + 2$ and $d(y) = n + 1$. So, in this case the contribution of these edges to the Randić index is

$$\zeta_5 = \sum_{i=1}^{t-1} \left(\frac{n}{n+1} + \frac{n^i - n}{\sqrt{(n+1)(n+2)}} \right)$$
$$= \frac{(t-1)n}{n+1} + \frac{n(n^{t-1} - 1)}{(n-1)\sqrt{(n+1)(n+2)}} - \frac{(t-1)n}{\sqrt{(n+1)(n+2)}}.$$

(6) $x \in A_t$ and $y \in V_t$. In this case, there are n edges $\{x, y\}$ where y is an extreme vertex of $S(K_n, t)$ for which $d(x) = n + 1$ and $d(y) = n$. For the remaining $n^t - n$ edges we have $d(x) = d(y) = n + 1$ and, as a consequence, the contribution of these edges to the Randić index is

$$\zeta_6 = \sqrt{\frac{n}{n+1}} + \frac{n^t - n}{n+1}.$$

(7) $x, y \in V_t$. There are $n(n - 1)$ edges $\{x, y\}$ where x is an extreme vertex of $S(K_n, t)$ and y is not, and for these vertices we have $d(x) = n$ and $d(y) = n + 1$. Also, we know that the size of $S(K_n, t)$ is $\frac{n^{t+1}-n}{2}$, so there are $\frac{n^{t+1}-n}{2} - n(n - 1)$ edges $\{x, y\}$ where nor x nor y are extreme vertices of $S(K_n, t)$ and for these vertices we have $d(x) = d(y) = n + 1$. Hence, the contribution of these edges to the Randić index is

$$\zeta_7 = (n-1)\sqrt{\frac{n}{n+1}} + \frac{n^{t+1} - 2n^2 + n}{2(n+1)}.$$

Therefore, $R(P(K_n, t)) = \sum_{l=1}^{7} \zeta_l = \sum_{l=1}^{5} \alpha_l$. ■

Remark 8. *For any δ-regular graph G of order $n \ge 2$,*

$$R(P(G, 1)) = \sqrt{\frac{n}{\delta+1}} + \frac{n\delta}{2(\delta+1)}.$$

Proof. Since there is one vertex of degree n and n vertices of degree $\delta+1$, $P(G,1)$ has size $\frac{n(\delta+2)}{2}$. Hence, there are n edges $\{x,y\}$ where x has degree $d(x)=n$ and y has degree $d(y)=\delta+1$, and for the remaining $\frac{n(\delta+2)}{2}-n$ edges we have $d(x)=d(y)=\delta+1$. Therefore, the result follows as $R(P(G,1))=\frac{n}{\sqrt{n(\delta+1)}}+\frac{n\delta}{2(\delta+1)}$. ■

Given a graph H, the number of vertices of degree δ will be denoted by $g_{_H}(\delta)$.

Lemma 9. *For any triangle free δ-regular graph G of order n and any integer $t\geq 2$,*

(i) $g_{_{S(G,t)}}(\delta)=n^t-\frac{n\delta\left(n^{t-1}-1\right)}{n-1}$.

(ii) $g_{_{S(G,t)}}(\delta+1)=\frac{n\delta\left(n^{t-1}-1\right)}{n-1}$.

Proof. Notice that $S(G,t)$ is a semiregular graph of degrees δ and $\delta+1$. The set of vertices of degree $\delta+1$ in $S(G,2)$ is formed by the neighbours of the extreme vertices of $S(G,2)$, so $g_{_{S(G,t)}}(\delta+1)=n\delta$ and $g_{_{S(G,t)}}(\delta)=n^2-n\delta$.

For $t\geq 3$, any edge of $S(G,t)$ connecting two copies of $S(G,t-1)$ is formed by vertices of degree $\delta+1$ and, as a result, $g_{_{S(G,t)}}(\delta+1)=ng_{_{S(G,t-1)}}(\delta)+n\delta$. Therefore, for any $t\geq 2$ we have $g_{_{S(G,t)}}(\delta+1)=n^{t-1}\delta+n^{t-2}\delta+\cdots+n\delta=n\delta\left(\frac{n^{t-1}-1}{n-1}\right)$ and, as a consequence, $g_{_{S(G,t)}}(\delta)=n^t-n\delta\left(\frac{n^{t-1}-1}{n-1}\right)$. ■

Theorem 10. *For any triangle free δ-regular graph G of order $n\geq 2$ and any integer $t\geq 2$,*

$$R(P(G,t))=\sum_{i=1}^{7}\alpha_i,$$

where

$$\alpha_1=\frac{n}{\sqrt{n(\delta+2)}},\quad \alpha_2=\frac{n\delta}{2(\delta+2)},$$

$$\alpha_3=\frac{n\delta}{(1-n)\sqrt{(n+1)(\delta+3)}}\left(t-2-n\left(\frac{n^{t-2}-1}{n-1}\right)\right)+\frac{n^2(1-n^{t-2})}{(1-n)\sqrt{(n+1)(\delta+2)}}$$
$$+\frac{n\delta}{(1-n)\sqrt{(n+1)(\delta+2)}}\left(t-2-n\left(\frac{n^{t-2}-1}{n-1}\right)\right),$$

$$\alpha_4=\frac{n\delta^2(1-n^{t-2})}{(1-n)\sqrt{(\delta+2)(\delta+3)}}\left(1+\frac{1}{1-n}\right)+\frac{n}{(\delta+2)}\left(\frac{n\delta}{2}-\delta^2\right)\left(\frac{1-n^{t-2}}{1-n}\right)$$
$$+\frac{n\delta}{2(\delta+3)(1-n)}\left(t-2-n\left(\frac{1-n^{t-2}}{1-n}\right)\right)+\frac{n\delta^2}{(1-n)(\delta+3)}\left(t-2-\left(\frac{1-n^{t-2}}{1-n}\right)\right),$$

$$\alpha_5=\frac{n\delta}{(1-n)\sqrt{(n+1)(\delta+3)}}\left(t-1-\left(\frac{1-n^{t-1}}{1-n}\right)\right)$$

$$+\frac{n}{(1-n)\sqrt{(n+1)(\delta+2)}}\left(\left(1-n^{t-1}\right)\left(1+\frac{\delta}{1-n}\right)-\delta(t-1)\right),$$

$$\alpha_6=\frac{n\delta}{\sqrt{(\delta+2)(n+1)}}\left(\frac{1-n^{t-1}}{1-n}\right)+\left(n^t-n\delta\left(\frac{1-n^{t-1}}{1-n}\right)\right)\frac{1}{\sqrt{(\delta+1)(n+1)}}$$

and

$$\alpha_7=\left(n^{t-1}+\frac{n^{t-1}-n}{1-n}\right)\frac{\delta^2}{\sqrt{(\delta+1)(\delta+2)}}+\frac{n^{t-1}}{\delta+1}\left(\frac{n\delta}{2}-\delta^2\right)+$$

$$+\frac{n\delta}{2(\delta+2)}\left(\frac{1-n^{t-1}}{1-n}\right)+\frac{n\delta^2}{\delta+2}\left(\frac{1-n^{t-2}}{1-n}\right).$$

Proof. Let $d(x)$ be the degree of x in $P(G,t)$. We differentiate the following cases for any edge $\{x,y\}$ of $P(G,t)$.

1. $x=a_{1_1}$ and $y\in V_1$. In this case, there are n edges $\{x,y\}$ with $d(x)=n$ and $d(y)=\delta+2$. Then the contribution of these edges to the Randić index is equal to α_1.
2. $x,y\in V_1$. In these case, there are $\frac{n\delta}{2}$ edges $\{x,y\}$ with $d(x)=d(y)=\delta+2$. So, the contribution of these edges to the Randić index is equal to α_2.
3. $x\in A_i$ and $y\in V_i$ for $2\le i\le t-1$. In this case $d(x)=n+1$ and, by Lemma 9, there are $g_{S(G,i)}(\delta+1)=\frac{n\delta\left(n^{i-1}-1\right)}{n-1}$ edges $\{x,y\}$ where y have degree $d(y)=\delta+3$ and there are $g_{S(G,i)}(\delta)=n^i-\frac{n\delta\left(n^{i-1}-1\right)}{n-1}$ edges $\{x,y\}$ where $d(y)=\delta+2$. Thus, the contribution of these edges to the Randić index is equal to α_3, *i.e.,*

$$\frac{n\delta}{\sqrt{(n+1)(\delta+3)}}\sum_{i=2}^{t-1}\frac{n^{i-1}-1}{n-1}+\frac{1}{\sqrt{(n+1)(\delta+2)}}\sum_{i=2}^{t-1}\left(n^i-\frac{n\delta\left(n^{i-1}-1\right)}{n-1}\right)=\alpha_3.$$

4. $x,y\in V_i$, for $2\le i\le t-1$. By Lemma 2 there are $f_{S(G,i)}(\delta,\delta+1)=\left(n^{i-1}+\frac{n^{i-1}-n}{1-n}\right)\delta^2$ edges $\{x,y\}$ where $d(x)=\delta+2$ and $d(y)=\delta+3$, $f_{S(G,i)}(\delta,\delta)=\frac{n^{i-1}\delta}{2}(n-2\delta)$ edges $\{x,y\}$ where $d(x)=d(y)=\delta+2$ and $f_{S(G,i)}(\delta+1,\delta+1)=\frac{n\delta}{2}\left(\frac{1-n^{i-1}}{1-n}\right)+n\delta^2\left(\frac{1-n^{i-2}}{1-n}\right)$ edges where $d(x)=d(y)=\delta+3$. Hence, the contribution of these edges to the Randić index is equal to α_4, *i.e.,*

$$\frac{\delta^2}{\sqrt{(\delta+2)(\delta+3)}}\sum_{i=2}^{t-1}\left(n^{i-1}+\frac{n^{i-1}-n}{1-n}\right)+\frac{\delta(n-2\delta)}{2(\delta+2)}\sum_{i=2}^{t-1}n^{i-1}+$$

$$+\frac{1}{\delta+3}\sum_{i=2}^{t-1}\left(\frac{n\delta}{2}\left(\frac{1-n^{i-1}}{1-n}\right)+n\delta^2\left(\frac{1-n^{i-2}}{1-n}\right)\right)=\alpha_4.$$

5. $x \in A_{i+1}$ and $y \in V_i$ for $1 \le i \le t-1$. In this case $d(x) = n+1$ and, by Lemma 9, there are $g_{S(G,i)}(\delta+1) = \dfrac{n\delta\,(n^{i-1}-1)}{n-1}$ edges $\{x,y\}$ where y have degree $d(y) = \delta+3$ and there are $g_{S(G,i)}(\delta) = n^i - \dfrac{n\delta\,(n^{i-1}-1)}{n-1}$ edges $\{x,y\}$ where $d(y) = \delta+2$. Hence, the contribution of these edges to the Randić index is equal to α_5, *i.e.*,

$$\frac{n\delta}{\sqrt{(n+1)(\delta+3)}}\sum_{i=1}^{t-1}\frac{n^{i-1}-1}{n-1} + \frac{1}{\sqrt{(n+1)(\delta+2)}}\sum_{i=1}^{t-1}\left(n^i - \frac{n\delta\,(n^{i-1}-1)}{n-1}\right) = \alpha_5.$$

6. $x \in A_t$ and $y \in V_t$. As above $d(x) = n+1$ and, by Lemma 9, there are $g_{S(G,t)}(\delta+1) = \dfrac{n\delta\,(1-n^{t-1})}{1-n}$ edges $\{x,y\}$ where y have degree $d(y) = \delta+2$ and there are $g_{S(G,t)}(\delta) = n^t - \dfrac{n\delta\,(1-n^{t-1})}{1-n}$ edges $\{x,y\}$ where $d(y) = \delta+1$. Thus, the contribution of these edges to the Randić index is equal to α_6.

7. $x, y \in V_t$,. By Lemma 2 there are $f_{S(G,t)}(\delta,\delta+1) = \left(n^{t-1} + \dfrac{n^{t-1}-n}{1-n}\right)\delta^2$ edges $\{x,y\}$ where $d(x) = \delta+1$ and $d(y) = \delta+2$, $f_{S(G,t)}(\delta,\delta) = n^{t-1}\left(\dfrac{n\delta}{2} - \delta^2\right)$ edges $\{x,y\}$ where $d(x) = d(y) = \delta+1$ and $f_{S(G,t)}(\delta+1,\delta+1) = \dfrac{n\delta}{2}\left(\dfrac{1-n^{t-1}}{1-n}\right) + n\delta^2\left(\dfrac{1-n^{t-2}}{1-n}\right)$ edges where $d(x) = d(y) = \delta+2$. Hence, the contribution of these edges to the Randić index is equal to α_7.

According to the seven cases above, the result follows. ■

We can use Lemma 4 to obtain a formula for the Randić index of $P(G,t)$, where G is a bipartite semiregular graph. The drawback of presenting the result is that, in this case, the formula obtained following the procedure described in the proof of Theorem 10 is extremely large.

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