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On the Schultz Index of Thorn Graphs

Damir Vukičević,[1] Sonja Nikolić,[2] and Nenad Trinajstić [2]

[1] Department of Mathematics, University of Split, Teslina 12, HR–21000, Croatia
[2] The Rugjer Bošković Institute, P.O. Box 180, HR–10001 Zagreb, Croatia

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[1] Department of Mathematics, University of Split, Teslina 12, HR–21000, Croatia
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Abstract

Motivation. This report was motivated by recent papers of Bytautas, Bonchev and Klein, Bonchev and Klein on the Wiener index of a special class of graphs called thorn graphs and of several groups of authors on the relationship between of the Schultz index and Wiener index.

Method. Graph–theoretical and algebraic methodologies are used in this paper.

Results. Three theorems are given from which as corrolaries follow Schultz indices of thorn graphs, such as thorn paths (thorn rods, thorn trees), thorn cycles, and thorn stars.

Conclusions. Obtained formulas allow much easier calculation of Schultz indices for thorn graphs than the formula for the Schultz index based on the adjacency matrix, distance matrix and valency matrix of a graph.

Keywords. Schultz index; thorn cycles; thorn graphs; thorn paths; thorn rods; thorn stars; thorn trees.

1 INTRODUCTION

This report, in which we derived Schultz indices of thorn graphs, was motivated by a recent paper of Bonchev and Klein on the Wiener index of thorn graphs [1] and by their earlier paper together with Bytautas on generating mean Wiener indices of these graphs [2]. A thorn graph G_p can be generated from a connected graph G by attaching p new vertices to each vertex of G. We considered the following thorn graphs: thorn paths (thorn trees, thorn rods), thorn cycles and thorn stars. Schultz [3] has introduced in 1989 a graph–theoretical descriptor for characterizing alkanes by an integer. He named this descriptor the *molecular topological index* and denoted it by MTI. Later MTI became much better known under the name the *Schultz index* [4–6]. While Schultz in his initial paper only described MTI, von Knop and his group [7] gave the mathematical formulation of MTI in the same year (1989). The MTI is based on the adjacency ($n \times n$) matrix denoted as $A(G)$, the distance ($n \times n$) matrix denoted as $D(G)$ and the valency ($1 \times n$) matrix denoted as $Val(G)$ of a graph G, where n is the number of vertices in G. Since in the definition of MTI appears the distance

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* Correspondence author; E–mail: vukicevi@pmfst.hr.

matrix on which is based the Wiener number [8,9], it has been found that the Schultz index and the Wiener index are closely related quantities for trees and cycles [10–14]. The Schultz index has been shown to be a useful molecular descriptor in the design of molecules with desired properties [5,6,15]. Mathematical properties of MTI have also been studied [11–14]. Therefore, further studies on mathematical and computational properties of the Schultz index and on its relation to other molecular descriptors are desirable.

2 DEFINITIONS AND NOTATIONS

The following graph–theoretical definitions and notations will be used [4,16]. $V(G)$ and $E(G)$ denote, respectively, the set of vertices $\{v_1, v_2, \ldots, v_n\}$ and the set of edges $\{e_1, e_2, \ldots, e_n\}$ of a graph G. Symbol G_p^u (u stands for uniform distribution) denotes a thorn graph obtained from G by adding to each of its vertices p neighbors, G_p^s ($p \geq \Delta(G)$) denotes a graph obtained from G by adding to each of its vertices v_i exactly $p–d(v_i)$ new neighbors and G^d will stand for a graph obtained from G by adding to each of its vertices v_i exactly $d(v_i)$ new neighbors. Note, $\Delta(G)$ denotes the maximal vertex–degree in G. $d_G(x)$ or $d(x)$ denotes the degree of a vertex x, whilst $dist_G(x,y)$ or $dist(x,y)$ is the graph–theoretical distance between the vertices x and y. The largest whole number not larger than x is denoted by $\lfloor x \rfloor$ and the smallest whole number not smaller than x is denoted by $\lceil x \rceil$.

We will use three auxiliary matrices, the $(n\times n)$ identity matrix I_n, the $(1\times n)$ row matrix u_n and the $(n\times n)$ square matrix J_n, both containing all elements equal to unity.

The valency matrix $Val(G)$ of a graph G is given by:

$$Val(\mathrm{G}) = [d(v_1)\ d(v_2)\ \ldots\ d(v_n)]$$

and the Schultz index $MTI(G)$ of a graph G is then defined as:

$$MTI(\mathrm{G}) = Val(\mathrm{G})\ B(\mathrm{G})\ u^{\tau}(\mathrm{G})$$

where $B(\mathrm{G})$ is the sum–matrix:

$$B(\mathrm{G}) = \mathrm{A}(\mathrm{G}) + D(\mathrm{G}).$$

Since we will mention the Gordon–Scantlebury index $S(G)$ [17] and the Wiener index $W(G)$ [18] of a graph G, we give below their definitions:

$$S(G) = \sum_i (L_3)_i = (1/2)\sum_{v\in V}\left[d(v)(d(v)-1)\right]$$

$$W(G) = (1/2)\sum_{ij}\left[D(G)\right]_{ij}$$

where L_3 is the number of paths of the length 2.

3 THORN GRAPHS

Theorem 1 Let G be any graph and G^* be the corresponding thorn graph obtained by attaching p new vertices to each vertex, then we have

$$MTI\left(G^*\right)=\begin{pmatrix}\left(p+1\right)\cdot MTI\left(G\right)-2p\cdot S\left(G\right)+\left(p^2-p\right)\cdot v\left(G\right)+2p\cdot e\left(G\right)\\ +2p\cdot v\left(G\right)\cdot e\left(G\right)+\left(4p^2+4p\right)\cdot W\left(G\right)+\left(3p^2+p\right)\cdot v\left(G\right)^2\end{pmatrix}$$

Proof: We make use of the formula for the Schultz index given above

$$\begin{aligned}&MTI\left(G^*\right)\\ &=Val\left(G^*\right)\cdot B\left(G\right)\cdot u^{\tau}_{(p+1)n}\\ &=\left[Val\left(G\right)+p\cdot u_n \quad u_{pn}\right]\cdot\left(A\left(G^*\right)+D\left(G^*\right)\right)\cdot u^{\tau}_{(p+1)n}\\ &=\left[Val\left(G\right)+p\cdot u_n \quad u_{pn}\right]\cdot A\left(G^*\right)\cdot u^{\tau}_{(p+1)n}+\left[Val\left(G\right)+p\cdot u_n \quad u_{pn}\right]\cdot D\left(G^*\right)\cdot u^{\tau}_{(p+1)n}\end{aligned}$$

$$\left(\begin{array}{l}\left[Val\left(G\right)+p\cdot u_n \quad u_n \quad u_n \quad \cdots \quad u_n\right]\cdot\begin{bmatrix}A\left(G\right) & I_n & I_n & \cdots & I_n\\ I_n & 0 & 0 & \cdots & 0\\ I_n & 0 & 0 & \cdots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ I_n & 0 & 0 & \cdots & 0\end{bmatrix}\cdot\begin{bmatrix}u_n^{\tau}\\ u_n^{\tau}\\ u_n^{\tau}\\ \vdots\\ u_n^{\tau}\end{bmatrix}+\left[Val\left(G\right)+p\cdot u_n \quad u_n \quad u_n \quad \cdots \quad u_n\right]\cdot\\ \begin{bmatrix}D\left(G\right) & D\left(G\right)+J_n & D\left(G\right)+J_n & \cdots & D\left(G\right)+J_n\\ D\left(G\right)+J_n & D\left(G\right)+2J_n-I_n & D\left(G\right)+2J_n & \cdots & D\left(G\right)+2J_n\\ D\left(G\right)+J_n & D\left(G\right)+2J_n & D\left(G\right)+2J_n-I_n & \cdots & D\left(G\right)+2J_n\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ D\left(G\right)+J_n & D\left(G\right)+2J_n & D\left(G\right)+2J_n & \cdots & D\left(G\right)+2J_n-I_n\end{bmatrix}\cdot\begin{bmatrix}u_n^{\tau}\\ u_n^{\tau}\\ u_n^{\tau}\\ \vdots\\ u_n^{\tau}\end{bmatrix}\end{array}\right)$$

$$=\left(\begin{array}{l}\underline{\left(\left(Val\left(G\right)+p\cdot u_n\right)\cdot A\left(G\right)\cdot u_n^{\tau}\right)}+\underline{\underline{p\cdot\left(u_n\cdot I_n\cdot u_n^{\tau}\right)}}+\underline{\underline{\underline{p\cdot\left(\left(Val\left(G\right)+p\cdot u_n\right)\cdot I_n\cdot u_n^{\tau}\right)}}}+\\ \underline{\left(p+1\right)\cdot\left(\left(Val\left(G\right)+p\cdot u_n\right)\cdot D\left(G\right)\cdot u_n^{\tau}\right)}+\underline{\underline{\underline{\underline{p\cdot\left(\left(Val\left(G\right)+p\cdot u_n\right)\cdot J_n\cdot u_n^{\tau}\right)}}}}+\underline{\underline{\underline{\underline{\underline{\left(p^2+p\right)\cdot\left(u_n\cdot D\left(G\right)\cdot u_n^{\tau}\right)}}}}}+\\ +\underline{\underline{\underline{\underline{\underline{\underline{\left(2p^2+p\right)\cdot\left(u_n\cdot J_n\cdot u_n^{\tau}\right)}}}}}}-\underline{2p\cdot\left(u_n\cdot I_n\cdot u_n^{\tau}\right)}\end{array}\right)$$

$$=\left(\begin{array}{l}\underline{\left(p+1\right)\cdot MTI\left(G\right)}-\underline{p\cdot\left(Val\left(G\right)\cdot A\left(G\right)\cdot u_n^{\tau}\right)}+\underline{p\cdot u_n\cdot A\left(G\right)\cdot u_n^{\tau}}+\underline{\left(p+1\right)\cdot p\cdot\left(u_n\cdot D\left(G\right)\cdot u_n^{\tau}\right)}\\ -\underline{\underline{p\cdot v\left(G\right)}}+\underline{\underline{4p\cdot e\left(G\right)}}+\underline{\underline{p^2v\left(G\right)}}+\underline{\underline{\underline{2p\cdot v\left(G\right)\cdot e\left(G\right)}}}+\underline{\underline{\underline{p^2v\left(G\right)^2}}}+\underline{\underline{\underline{\left(2p^2+2p\right)\cdot W\left(G\right)}}}+\underline{\underline{\underline{\underline{\left(2p^2+p\right)\cdot v\left(G\right)^2}}}}\end{array}\right)$$

$$=\begin{pmatrix}\left(p+1\right)\cdot MTI\left(G\right)-p\cdot\sum_{i=1}^{v(G)}d_i^{\,2}+\left(p^2-p\right)\cdot v\left(G\right)+4p\cdot e\left(G\right)+\\ +2p\cdot v\left(G\right)\cdot e\left(G\right)+\left(4p^2+4p\right)\cdot W\left(G\right)+\left(3p^2+p\right)\cdot v\left(G\right)^2\end{pmatrix}$$

$$=\begin{pmatrix}\left(p+1\right)\cdot MTI\left(G\right)-p\cdot\sum_{i=1}^{v(G)}\left(d_i^{\,2}-d_i\right)-p\cdot 2\cdot e\left(G\right)+\left(p^2-p\right)\cdot v\left(G\right)+4p\cdot e\left(G\right)+\\ +2p\cdot v\left(G\right)\cdot e\left(G\right)+\left(4p^2+4p\right)\cdot W\left(G\right)+\left(3p^2+p\right)\cdot v\left(G\right)^2\end{pmatrix}$$

$$=\begin{pmatrix}\left(p+1\right)\cdot MTI\left(G\right)-2p\cdot S\left(G\right)+\left(p^2-p\right)\cdot v\left(G\right)+2p\cdot e\left(G\right)\\ +2p\cdot v\left(G\right)\cdot e\left(G\right)+\left(4p^2+4p\right)\cdot W\left(G\right)+\left(3p^2+p\right)\cdot v\left(G\right)^2\end{pmatrix}$$

4 THORN CYCLES

C_n denotes a cycle with n vertices. From the above follows:

Corollary 2 Let $n \geq 3$. Then

$$MTI\left(\left(C_n\right)_p^u\right) = \left(\left(2p^2+3p\right)\cdot n^2 + \left(p^2+3p\right)n + 4n + \left(4p^2+8p+4\right)\cdot\left(\frac{n}{2}\cdot\left\lfloor\frac{n}{2}\right\rfloor\cdot\left\lceil\frac{n}{2}\right\rceil\right)\right).$$

Proof: Note that

$$v\left(C_n\right) = n$$

$$e\left(C_n\right) = n$$

$$S\left(C_n\right) = n$$

$$W\left(C_n\right) = \begin{cases} \frac{1}{2}\cdot n\cdot\left(2\cdot\frac{\frac{n}{2}\cdot\left(\frac{n}{2}-1\right)}{2}+\right), & n \text{ is even} \\ \frac{1}{2}\cdot n\cdot\left(2.\frac{\left\lfloor\frac{n}{2}\right\rfloor\cdot\left(\left\lfloor\frac{n}{2}\right\rfloor+1\right)}{2}\right), & n \text{ is odd} \end{cases}$$

$$= \begin{cases} \frac{1}{2}\cdot n\cdot\left(\frac{n}{2}\cdot\frac{n}{2}\right), & n \text{ is even} \\ \frac{1}{2}\cdot n\cdot\left(\left\lfloor\frac{n}{2}\right\rfloor.\left(\left\lfloor\frac{n}{2}\right\rfloor+1\right)\right), & n \text{ is odd} \end{cases}$$

$$= \frac{n}{2}\cdot\left\lfloor\frac{n}{2}\right\rfloor\cdot\left\lceil\frac{n}{2}\right\rceil.$$

$$MTI\left(C_n\right) = 4n + 4\cdot W\left(C_n\right) = 4n + 2n\cdot\left\lfloor\frac{n}{2}\right\rfloor\cdot\left\lceil\frac{n}{2}\right\rceil$$

From the last theorem follows that

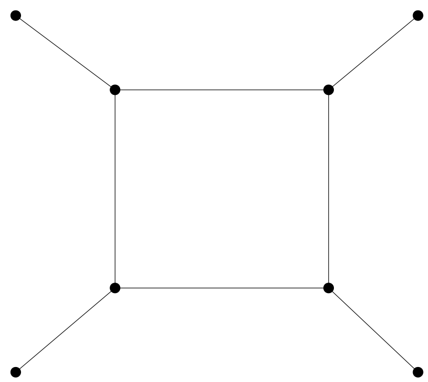
$$MTI\left(\left(C_n\right)_p^u\right) = \begin{pmatrix} \left(p+1\right)\cdot MTI\left(C_n\right) - 2p\cdot S\left(C_n\right) + \left(p^2-p\right)\cdot v\left(C_n\right) + 2p\cdot e\left(C_n\right) \\ +2p\cdot v\left(C_n\right)\cdot e\left(C_n\right) + \left(4p^2+4p\right)\cdot W\left(C_n\right) + \left(3p^2+p\right)\cdot v\left(C_n\right)^2 \end{pmatrix}$$

$$= \begin{pmatrix} \left(p+1\right)\cdot\left(4n+2n\cdot\left\lfloor\frac{n}{2}\right\rfloor\cdot\left\lceil\frac{n}{2}\right\rceil\right) - 2p\cdot n + \left(p^2-p\right)\cdot n + 2p\cdot n + \\ 2p\cdot n^2 + \left(4p^2+4p\right)\cdot\left(\frac{n}{2}\cdot\left\lfloor\frac{n}{2}\right\rfloor\cdot\left\lceil\frac{n}{2}\right\rceil\right) + \left(3p^2+p\right)\cdot n^2 \end{pmatrix}$$

$$= \left(\left(3p^2+3p\right)\cdot n^2 + \left(p^2+3p+4\right)n + \left(4p^2+8p+4\right)\cdot\left(\frac{n}{2}\cdot\left\lfloor\frac{n}{2}\right\rfloor\cdot\left\lceil\frac{n}{2}\right\rceil\right)\right).$$

Let us demonstrate the use of this formula with one example:

Example 3 Let us calculate $MTI\left(\left(C_4\right)_1^u\right)$.



$\left(C_4\right)_1^u$

Using the last Corollary, we get

$$.MTI\left(\left(C_4\right)_1^u\right) = \left(\left(3\cdot 1^2 + 3\cdot 1\right)\cdot 4^2 + \left(1^2 + 3\cdot 1 + 4\right)\cdot 4 + \left(4\cdot 1^2 + 8\cdot 1 + 4\right)\cdot\left(\frac{4}{2}\cdot\left\lfloor\frac{4}{2}\right\rfloor\cdot\left\lceil\frac{4}{2}\right\rceil\right)\right) = 256.$$

On the other hand, we can directly calculate $MTI\left(\left(C_4\right)_1^u\right)$ using the formula for the Schultz index given above:

$$MTI\left(\left(C_4\right)_1^u\right) = \begin{bmatrix}3 & 3 & 3 & 3 & 1 & 1 & 1 & 1\end{bmatrix}\cdot\begin{bmatrix}0 & 2 & 2 & 2 & 2 & 2 & 3 & 2\\ 2 & 0 & 2 & 2 & 2 & 2 & 2 & 3\\ 2 & 2 & 0 & 2 & 3 & 2 & 2 & 2\\ 2 & 2 & 2 & 0 & 2 & 3 & 2 & 2\\ 2 & 2 & 3 & 2 & 0 & 3 & 4 & 3\\ 2 & 2 & 2 & 3 & 3 & 0 & 3 & 4\\ 3 & 2 & 2 & 2 & 4 & 3 & 0 & 3\\ 2 & 3 & 2 & 2 & 3 & 4 & 3 & 0\end{bmatrix}\cdot\begin{bmatrix}1\\1\\1\\1\\1\\1\\1\\1\end{bmatrix} = 256.$$

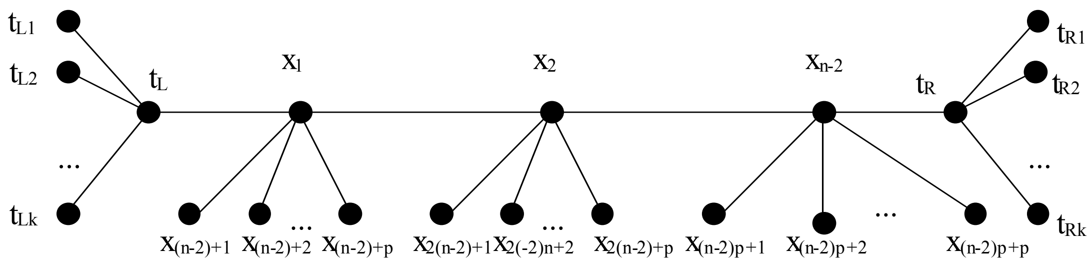
5 THORN PATHS

P_n stands for a path with n vertices, while $P_{n,p,k}$ denotes a tree obtained from P_n by adding p neighbors to each of its nonterminal vertices and k neighbors to each of its terminal vertices. Let us now prove the following theorem.

Theorem 4 Let $n \geq 2$ and let p and k be any nonnegative numbers. Then we have

$$MTI\left(P_{n,p,k}\right)==\left(\begin{array}{l}-6+10k^2+\dfrac{13n}{3}+4k^2n-n^2+4kn^2+\dfrac{2n^3}{3}-8p-16kp+\dfrac{14np}{3}-3n^2p+\\+4kn^2p+\dfrac{4n^3p}{3}+6p^2-\dfrac{11np^2}{3}-n^2p^2+\dfrac{2n^3p^2}{3}\end{array}\right).$$

Proof: Denote vertices of $P_{n,p,k}$ as on the following branched tree



Denote

$$T=\left\{t_L,t_R,t_{L_1},t_{L_2},\ldots,t_{L_k},t_{R_1},t_{R_2},\ldots,t_{R_k}\right\}$$
$$T_L=\left\{t_{L_1},t_{L_2},\ldots,t_{L_k}\right\}$$
$$T_R=\left\{t_{R_1},t_{R_2},\ldots,t_{R_k}\right\}$$
$$P'=\left\{x_1,x_2,\ldots,x_{n-1}\right\}$$
$$P''=\left\{x_{(n-2)+1},\ldots,x_{(n-2)(p+1)}\right\}.$$

Then we have

$$MTI\left(P_{n,p,k}\right)=$$
$$=Val\left(P_{n,p,k}\right)\cdot B\left(P_{n,p,k}\right)\cdot u^{\tau}_{n+(n-2)p+2k}$$
$$=Val\left(P_{n,p,k}\right)\cdot A\left(P_{n,p,k}\right)\cdot u^{\tau}_{n+(n-2)p+2k}+Val\left(P_{n,p,k}\right)\cdot D\left(P_{n,p,k}\right)\cdot u^{\tau}_{n+(n-2)p+2k} \qquad (1)$$
$$=\left(\sum_{v\in V\left(P_{n,p,k}\right)}d(v)^2+\sum_{\substack{x,y\in V\left(P_{n,p,k}\right)\\(x\in T)\vee(y\in T)}}dist(x,y)\big(d(x)+d(y)\big)+\sum_{\substack{x,y\in V\left(P_{n,p,k}\right)\\(x\notin T)\wedge(y\notin T)}}dist(x,y)\big(d(x)+d(y)\big)\right). \qquad (1)$$

Note that

$$\sum_{v\in V\left(P_{n,p,k}\right)}d(v)^2=(n-2)\cdot p+2k+(n-2)\cdot(p+2)^2+2(k+1)^2. \qquad (2) \qquad (2)$$

Now, let us calculate $\sum_{\substack{x,y\in V\left(P_{n,p,k}\right)\\(x\in T)\vee(y\in T)}}dist(x,y)\cdot\big(d(x)+d(y)\big).$

Two cases can be distinguished:

CASE 1: $n \geq 3$.

$$\sum_{\substack{x,y\in V(P_{n,p,k})\\ (x\in T)\vee(y\in T)}} dist(x,y)\cdot\left(d(x)+d(y)\right)=$$

$$=\begin{pmatrix} dist(t_L,t_R)\left(d(t_L)+d(t_R)\right)+\sum_{\substack{x\in T_L\\ y\in T_R}} dist(x,y)\left(d(x)+d(y)\right)+ \\ +\sum_{x\in T_L} dist(x,t_R)\left(d(x)+d(t_R)\right)+\sum_{x\in T_R} dist(x,t_R)\left(d(x)+d(t_R)\right)+ \\ +2\cdot\sum_{x,y\in T_L} dist(x,y)\left(d(x)+d(y)\right)+ \\ +\sum_{x\in P'} dist(x,t_R)\left(d(x)+d(t_R)\right)+\sum_{x\in P''} dist(x,t_R)\left(d(x)+d(t_R)\right)+ \\ +\sum_{\substack{x\in T_L\\ y\in P'}} dist(x,y)\left(d(x)+d(y)\right)+\sum_{\substack{x\in T_L\\ y\in P''}} dist(x,y)\left(d(x)+d(y)\right) \end{pmatrix}$$

$$=\begin{pmatrix} (n-1)\cdot 2(k+1)+k\cdot k\cdot(n+1)\cdot 2+ \\ 2\cdot k\cdot n\cdot(k+1)+2\cdot k\cdot 1\cdot(k+2)+ \\ +2\cdot\frac{k\cdot(k-1)}{2}\cdot 2\cdot 2+ \\ +2\cdot\sum_{i=1}^{n-2}\left[i\cdot(k+3+p)\right]+2p\cdot\sum_{i=2}^{n-1}\left[\left(i\cdot(k+2)\right)\right]+ \\ +2\cdot k\cdot\sum_{i=2}^{n-1}\left[i\cdot(3+p)\right]+2pk\cdot\sum_{i=3}^{n}\left[i\cdot 2\right] \end{pmatrix}$$

$$=4-6k+8k^2-7n+4k^2n+3n^2+4kn^2-2p-16kp-5np+3n^2p+4kn^2p$$

CASE 2: $n = 2$.

$$\sum_{\substack{x,y\in V(P_{n,p,k})\\ (x\in T)\vee(y\in T)}} dist(x,y)\cdot\left(d(x)+d(y)\right)=$$

$$=\begin{pmatrix} dist(t_L,t_R)\left(d(t_L)+d(t_R)\right)+\sum_{\substack{x\in T_L\\ y\in T_R}} dist(x,y)\left(d(x)+d(y)\right)+ \\ +\sum_{x\in T_L} dist(x,t_R)\left(d(x)+d(t_R)\right)+\sum_{x\in T_R} dist(x,t_R)\left(d(x)+d(t_R)\right)+ \\ +2\cdot\sum_{x,y\in T_L} dist(x,y)\left(d(x)+d(y)\right)+ \end{pmatrix}$$

$$=\begin{pmatrix} (n-1)\cdot 2(k+1)+k\cdot k\cdot(n+1)\cdot 2+ \\ 2\cdot k\cdot n\cdot(k+1)+2\cdot k\cdot 1\cdot(k+2)+ \\ +2\cdot\dfrac{k\cdot(k-1)}{2}\cdot 2\cdot 2 \end{pmatrix}$$

Simple calculation shows that this is also equal to

$$4-6k+8k^2-7n+4k^2n+3n^2+4kn^2-2p-16kp-5np+3n^2p+4kn^2p$$

Therefore, in any case, we have

$$\sum_{\substack{x,y\in V(P_{n,p,k}) \\ (x\in T)\vee(y\in T)}} dist(x,y)\cdot(d(x)+d(y))= \\ =4-6k+8k^2-7n+4k^2n+3n^2+4kn^2-2p-16kp-5np+3n^2p+4kn^2p. \quad (3)$$

Now, let us find $\sum_{\substack{x,y\in V(P_{n,p,k}) \\ (x\notin T)\wedge(y\notin T)}} dist(x,y)(d(x)+d(y))$.

Again, one can distinguish two cases:

CASE 1: $n\geq 3$.

$$\sum_{\substack{x,y\in V(P_{n,p,k}) \\ (x\notin T)\wedge(y\notin T)}} dist(x,y)(d(x)+d(y))=$$

$$=\left(\begin{matrix} \left[(p+2)u_{n-2}\quad u_{p(n-2)}\right]\cdot \\ \begin{bmatrix} D(P_{n-2}) & D(P_{n-2})+J_{n-2} & D(P_{n-2})+J_{n-2} & \cdots & D(P_{n-2})+J_{n-2} \\ D(P_{n-2})+J_{n-2} & D(P_{n-2})+2J_{n-2}-2I_{n-2} & D(P_{n-2})+2J_{n-2} & \cdots & D(P_{n-2})+2J_{n-2} \\ D(P_{n-2})+J_{n-2} & D(P_{n-2})+2J_{n-2} & D(P_{n-2})+2J_{n-2}-2I_{n-2} & \cdots & D(P_{n-2})+2J_{n-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ D(P_{n-2})+J_{n-2} & D(P_{n-2})+2J_{n-2} & D(P_{n-2})+2J_{n-2} & \cdots & D(P_{n-2})+2J_{n-2}-2I_{n-2} \end{bmatrix} \\ u^{\tau}_{(n-2)(p+1)} \end{matrix}\right) \quad (4)$$

$$=\begin{pmatrix} (p+1)\cdot((p+2)u_{n-2}\cdot D(P_{n-2})\cdot u^{\tau}_{n-2})+p((p+2)u_{n-2}\cdot J_{n-2}\cdot u^{\tau}_{n-2})+ \\ +(p^2+p)\cdot(u_{n-2}\cdot D(P_{n-2})\cdot u^{\tau}_{n-2})+(2p^2+p)\cdot(u_{n-2}\cdot J_{n-2}\cdot u^{\tau}_{n-2})- \\ -2p\cdot(u_{n-2}\cdot I_{n-2}\cdot u^{\tau}_{n-2}) \end{pmatrix}$$

$$=(2p^2+4p+2)\cdot(u_{n-2}\cdot D(P_{n-2})\cdot u^{\tau}_{n-2})+(3p^2+3p)\cdot(n-2)^2-2p\cdot(n-2). \quad (4)$$

Now, let us calculate $u_{n-2}\cdot D(P_{n-2})\cdot u^{\tau}_{n-2}$. One can distinguish two subcases:

SUBCASE 1.1: *n* is odd.

$$u_{n-2}\cdot D\left(P_{n-2}\right)\cdot u_{n-2}^{\tau}=\begin{cases}0, & n=3\\ \left(n-2\right)\cdot 2\cdot\sum_{i=1}^{\left\lfloor\frac{n-2}{2}\right\rfloor} i+2\cdot\sum_{i=1}^{\left\lfloor\frac{n-2}{2}\right\rfloor}\sum_{j=1}^{i}\left(2j-1\right), & n>3\end{cases}$$

$$=\begin{cases}0, & n=3\\ \frac{n^3}{3}-2n^2+\frac{11n}{3}-2, & n>3\end{cases}$$

$$=\frac{n^3}{3}-2n^2+\frac{11n}{3}-2.$$

SUBCASE 1.2: *n* is even

$$u_{n-2}\cdot D\left(P_{n-2}\right)\cdot u_{n-2}^{\tau}=\begin{cases}2, & n=4\\ \left(n-2\right)\left(\sum_{i=1}^{\frac{n-2}{2}} i+\sum_{i=1}^{\frac{n-2}{2}} i\right)+2\cdot\sum_{i=1}^{\frac{n-2}{2}-1}\sum_{j=1}^{i}2j, & n>4\end{cases}$$

$$=\begin{cases}0, & n=4\\ \frac{n^3}{3}-2n^2+\frac{11n}{3}-2, & n>4\end{cases}$$

$$=\frac{n^3}{3}-2n^2+\frac{11n}{3}-2.$$

So, in any case we have

$$u_{n-2}\cdot D\left(P_{n-2}\right)\cdot u_{n-2}^{\tau}=\frac{n^3}{3}-2n^2+\frac{11n}{3}-2. \tag{5}$$

Putting (5) in (4), we get

$$\sum_{\substack{x,y\in V\left(P_{n,p,k}\right)\\ \left(x\notin T\right)\wedge\left(y\notin T\right)}} dist\left(x,y\right)\left(d\left(x\right)+d\left(y\right)\right)=$$

$$=\left(2p^2+4p+2\right)\cdot\left(\frac{n^3}{3}-2n^2+\frac{11n}{3}-2\right)+\left(3p^2+3p\right)\cdot\left(n-2\right)^2-2p\cdot\left(n-2\right).$$

CASE 2: $n=2$

Evidently:

$$\sum_{\substack{x,y\in V\left(P_{n,p,k}\right)\\ \left(\left(x\notin T\right)\wedge\left(y\notin T\right)\right)}} dist\left(x,y\right)\left(d\left(x\right)+d\left(y\right)\right)=0$$

Therefore,

$$\sum_{\substack{x,y\in V(P_{n,p,k})\\ ((x\notin T)\wedge(y\notin T))}} dist(x,y)\big(d(x)+d(y)\big)=0=$$
$$=\left(2p^2+4p+2\right)\cdot\left(\frac{n^3}{3}-2n^2+\frac{11n}{3}-2\right)+\left(3p^2+3p\right)\cdot(n-2)^2-2p\cdot(n-2)$$

So, in any case, we have

$$\sum_{\substack{x,y\in V(P_{n,p,k})\\ (x\notin T)\wedge(y\notin T)}} dist(x,y)\big(d(x)+d(y)\big)=$$
$$=\left(2p^2+4p+2\right)\cdot\left(\frac{n^3}{3}-2n^2+\frac{11n}{3}-2\right)+\left(3p^2+3p\right)\cdot(n-2)^2-2p\cdot(n-2). \tag{6}$$

Introducing (2), (3) and (6) into (1), we get

$$MTI(P_{n,p,k})=$$
$$=\left(\begin{array}{l}\left((n-2)\cdot p+2k+(n-2)\cdot(p+2)^2+2(k+1)^2\right)+\\ \left(4-6k+8k^2-7n+4k^2n+3n^2+4kn^2-2p-16kp-5np+3n^2p+4kn^2p\right)+\\ \left(2p^2+4p+2\right)\cdot\left(\frac{n^3}{3}-2n^2+\frac{11n}{3}-2\right)+\left(3p^2+3p\right)\cdot(n-2)^2-2p\cdot(n-2)\end{array}\right)$$
$$=\left(\begin{array}{l}-6+10k^2+\frac{13n}{3}+4k^2n-n^2+4kn^2+\frac{2n^3}{3}-4p-16kp+\frac{2np}{3}-2n^2p+\\ +4kn^2p+\frac{4n^3p}{3}+6p^2-\frac{11np^2}{3}-n^2p^2+\frac{2n^3p^2}{3}\end{array}\right).$$

Now, we can use this general theorem to find molecular topological indices for some more special families of paths.

Corollary 5 Let $n\geq 2$ and let *p* and *k* be any nonnegative numbers. Then, we have

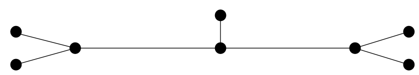
$$MTI(P_{n,p,p+1})=4+\frac{25n}{3}+3n^2+\frac{2n^3}{3}-4p+\frac{38np}{3}+5n^2p+\frac{4n^3p}{3}+\frac{np^2}{3}+3n^2p^2+\frac{2n^3p^2}{3}.$$

Proof:

$$MTI(P_{n,p,p+1})=$$
$$=\left(\begin{array}{l}-6+10(p+1)^2+\frac{13n}{3}+4(p+1)^2n-n^2+4(p+1)n^2+\frac{2n^3}{3}-4p-16(p+1)p+\\ \frac{2np}{3}-2n^2p+4(p+1)n^2p+\frac{4n^3p}{3}+6p^2-\frac{11np^2}{3}-n^2p^2+\frac{2n^3p^2}{3}\end{array}\right)$$
$$=4+\frac{25n}{3}+3n^2+\frac{2n^3}{3}+\frac{26np}{3}+6n^2p+\frac{4n^3p}{3}+\frac{np^2}{3}+3n^2p^2+\frac{2n^3p^2}{3}.$$

Let the use illustrate of this with one example.

Example 6 Let us calculate $MTI\left(P_{3,1,2}\right)$ for a simple thorn tree.



$P_{3,1,2}$

From the last Corollary, we get

$$MTI\left(P_{3,1,2}\right)=$$
$$4+\frac{25n}{3}+3n^2+\frac{2n^3}{3}+\frac{26np}{3}+6n^2p+\frac{4n^3p}{3}+\frac{np^2}{3}+3n^2p^2+\frac{2n^3p^2}{3}$$
$$=4+\frac{25\cdot 3}{3}+3\cdot 3^2+\frac{2\cdot 3^3}{3}+\frac{26\cdot 3\cdot 1}{3}+6\cdot 3^2\cdot 1+\frac{4\cdot 3^3\cdot 1}{3}+\frac{3\cdot 1^2}{3}+3\cdot 3^2\cdot 1^2+\frac{2\cdot 3^3\cdot 1^2}{3}$$
$$=236.$$

On the other hand, we can directly calculate $MTI(P_{3,1,2})$ using the original Schultz formula, given above:

$$MTI\left(P_{3,1,2}\right)=\begin{bmatrix}3 & 3 & 3 & 1 & 1 & 1 & 1 & 1\end{bmatrix}\cdot\begin{bmatrix}0&2&2&2&2&3&3&2\\2&0&2&2&2&2&2&2\\2&2&0&3&3&2&2&2\\2&2&3&0&2&4&4&3\\2&2&3&2&0&4&4&3\\3&2&2&4&4&0&2&3\\3&2&2&4&4&2&0&3\\2&2&2&3&3&3&3&0\end{bmatrix}\cdot\begin{bmatrix}1\\1\\1\\1\\1\\1\\1\\1\end{bmatrix}=236.$$

There is another interesting Corollary that follows from Theorem 4.

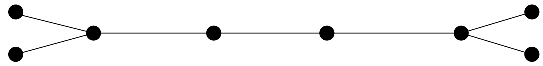
Corollary 7. Let p be any nonnegative number and $n\geq 2$. Then, we have

$$MTI\left(P_{n,0,k}\right)=\left(-6+10k^2+\frac{13n}{3}+4k^2n-n^2+4kn^2+\frac{2n^3}{3}\right).$$

Proof: Just put $p=0$ in Theorem 4.

Let us illustrate this Corollary with one example, too.

Example 8. Let us calculate $MTI\left(P_{4,0,2}\right)$ for a thorn rod [1].



$P_{4,0,2}$

From the last Corollary, we get

$$MTI\left(P_{4,0,2}\right)=-6+10\cdot 2^2+\frac{13\cdot 4}{3}+4\cdot 2^2\cdot 4-4^2+4\cdot 2\cdot 4^2+\frac{2\cdot 4^3}{3}=270.$$

On the other hand, we can directly calculate the $MTI(P_{4,0,2})$ using the Schultz formula:

$$MTI\left(P_{4,0,2}\right)=\begin{bmatrix}1 & 1 & 3 & 2 & 2 & 3 & 1 & 1\end{bmatrix}\cdot\begin{bmatrix}0 & 2 & 2 & 2 & 3 & 4 & 5 & 5\\ 2 & 0 & 2 & 2 & 3 & 4 & 5 & 5\\ 2 & 2 & 0 & 2 & 2 & 3 & 4 & 4\\ 2 & 2 & 2 & 0 & 2 & 2 & 3 & 3\\ 3 & 3 & 2 & 2 & 0 & 2 & 2 & 2\\ 4 & 4 & 3 & 2 & 2 & 0 & 2 & 2\\ 5 & 5 & 4 & 3 & 2 & 2 & 0 & 2\\ 5 & 5 & 4 & 3 & 2 & 2 & 2 & 0\end{bmatrix}\cdot\begin{bmatrix}1\\1\\1\\1\\1\\1\\1\\1\end{bmatrix}=270.$$

6 THORN STARS

We symbolize stars with S_n whilst $S_{n,p,k}$ denote thorn stars. $S_{n,p,k}$ can be obtained from S_n by adding p neighbors to the center of the star and k neighbors to its terminal vertices. Now, we prove the theorem 9.

Theorem 9 Let $n \geq 3$ and let p and k be any nonnegative numbers. Then, we have

$$MTI\left(S_{n,p,k}\right)=$$
$$=4+12k+10k^2-8n-22kn-17k^2n+4n^2+10kn^2+7k^2n^2-8p-10kp+7np+10knp+3p^2.$$

Proof:

$$MTI\left(S_{n,p,k}\right)=\left(\begin{array}{l}(n-1)\frac{k(k-1)}{2}\cdot 2\cdot(1+1)+\frac{(n-1)\cdot(n-2)}{2}\cdot 4\cdot k^2\cdot(1+1)+\\ +\frac{(n-1)\cdot(n-2)}{2}\cdot 2\cdot 2\cdot(k+1)+\frac{p\cdot(p-1)}{2}\cdot 2\cdot 2+\\ +(n-1)\cdot k\cdot 2\cdot(1+k+1)+(n-1)\cdot(n-2)\cdot k\cdot 3\cdot(1+k+1)+\\ +(n-1)\cdot k\cdot 2\cdot(p+n-1+1)+(n-1)\cdot k\cdot p\cdot 3\cdot(1+1)+\\ +(n-1)\cdot 1\cdot(k+1+n-1+p)+(n-1)\cdot p\cdot 2\cdot(k+1+1)+\\ p\cdot 1\cdot(n+p-1+1)\end{array}\right)$$
$$=4+12k+10k^2-8n-22kn-17k^2n+4n^2+10kn^2+7k^2n^2-8p-10kp+7np+10knp+3p^2.$$

From here follows

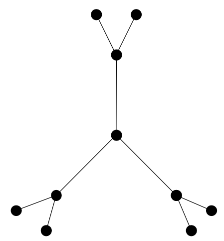
Corollary 10 Let $n \geq 3$ and let p and k be any nonnegative numbers. Then, we have

$$MTI\left(S_{n,p,k}\right)=4+12k+10k^2-8n-22kn-17k^2n+4n^2+10kn^2+7k^2n^2.$$

Proof: Just put $p = 0$ in the last theorem.

We also illustrate this Corollary with one example.

Example 11 Let us calculate $MTI\left(S_{4,0,2}\right)$.



$S_{4,0,2}$

From the last Corollary follows that

$$MTI\left(S_{4,0,2}\right) = 4 + 12 \cdot 2 + 10 \cdot 2^2 - 8 \cdot 4 - 22 \cdot 2 \cdot 4 - 17 \cdot 2^2 \cdot 4 + 4 \cdot 4^2 + 10 \cdot 2 \cdot 4^2 + 7 \cdot 2^2 \cdot 4^2 = 420.$$

On the other hand, we can directly calculate the $MTI(S_{4,0,2})$ using the formula for computing the Schultz index:

$$MTI\left(S_{4,0,2}\right) = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 3 & 3 & 3 & 3 \end{bmatrix} \cdot \begin{bmatrix} 0 & 2 & 4 & 4 & 4 & 4 & 2 & 3 & 3 & 2 \\ 2 & 0 & 4 & 4 & 4 & 4 & 2 & 3 & 3 & 2 \\ 4 & 4 & 0 & 2 & 4 & 4 & 3 & 2 & 3 & 2 \\ 4 & 4 & 2 & 0 & 4 & 4 & 3 & 2 & 3 & 2 \\ 4 & 4 & 4 & 4 & 0 & 2 & 3 & 3 & 2 & 2 \\ 4 & 4 & 4 & 4 & 2 & 0 & 3 & 3 & 2 & 2 \\ 2 & 2 & 3 & 3 & 3 & 3 & 0 & 2 & 2 & 2 \\ 3 & 3 & 2 & 2 & 3 & 3 & 2 & 0 & 2 & 2 \\ 3 & 3 & 3 & 3 & 2 & 2 & 2 & 2 & 0 & 2 \\ 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = 420.$$

7 CONCLUDING REMARKS

Comparison between our formulas and the related formulas for the Wiener number of thorn graphs [1] shows as expected that the Wiener number formulas are simpler. Formulas for the Wiener numbers of thorn graphs are given in terms of two parameters: n (the number of non–terminal vertices) and t>2 (the degree of non–terminal vertices higher than 2). Thus, the Wiener number of a thorn cycle denoted by us as $\left(C_4\right)_1^u$ and by Bonchev and Klein [1] as 3–thorn 4–cycle C_4;3 (C_n;t, n = 4, t = 3) is given by:

$$W(C_4;3) = [\, n^3(t-1)^2] / 8 + n(t-2)\,(\, nt - n - 1) = 60.$$

Similarly, the Wiener number of a thorn tree $P_{n,p,k}$ ($P_{3,1,2)}$ in our notation and $P_{n,t}$ ($P_{3,3}$) in the notation of Bonchev and Klein is:

$$W(P_{3,3}) = n\ (t-1)\ [(t-1)\ (n-1)\ (n+7) + 6\ (t+1)]/6 + 1 = 65.$$

The Wiener number of the thorn rod $P_{n,t}$ ($P_{4,3}$) in the Bonchev–Klein notation or $P_{n,p,p+1}$ ($P_{4,0,2}$ in our notation:

$$W(P_{4,3}) = (n^3 - n)/6 + (t-1)^2\ (n+3) + (t-1)\ (n^2 + n - 2) = 74.$$

Finally, the Wiener number of the in our thorn star $S_{k,t}$ ($S_{3,3}$), where $k = n - 1$, that is the number of star–arms (this thorn star is denoted by us $S_{4,0,2}$):

$$W(S_{3,3}) = k\ t\ (2\ k\ t - k - t + 1) = 117.$$

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