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The most private features of the topological index

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§ 1 Introduction

In early May of 2018 I got an astonishing e-mail from Turkey mathematician, Dr. Süleyman Ediz, asking to write an essay to a new journal MATI to be dedicated solely to those papers dealing with the mathematical aspects of the topological index (TI).

This is the most honorable and kindest offer from the group of distinguished scholars who are taking care of my beloved son bestowed to me nearly half a century ago. However, after to-and-fro net surfing I happened to know that these ladies and gentlemen don't seem to know the detailed birth and growth history of my son and his family. Then I decided to let them know the most private features of TI and the family talk around him including his godfather as honestly as I can, of course, within the scope of a scientific paper.

§ 2 Personal history of Haruo Hosoya (HH) related to TI

In 1936[*1] HH was born in Kamakura, an old capital town of Japan in 12th century, which is located to the 50 km south of Tokyo. He entered Univ. of Tokyo in 1955 to study chemistry, and in 1964 took the degree of Doctor of Science for "the research on the structure of reactive intermediates and reaction mechanism" under Prof. Saburo Nagakura. During his under-graduate age HH happened to estimate the boiling points of octane isomers reasonably well with ρ=0.942 using his own naïve conjecture. The detailed story about it is documented in his memoir "The topological index *Z* before and after 1971" [1]. However, this study is nothing related to his doctoral thesis and also to the biophysical study of vision research performed in Univ. of Michigan as a post-doctoral fellow under the direction of Prof. John Platt during 1967 and 1968.

Ironically enough, although Platt who worked with the Nobel Laureate Robert Mulliken in Chicago was the only scientist that realized the importance of the "pass number *w*" of Harry Wiener proposed in 1947 [2,3], HH did not know anything about the graph theory nor the papers by these pioneers in QSAR study during his one-year stay in Ann Arbor.

In the spring of 1969 HH became associate professor of chemistry in Ochanomizu Univ. in Tokyo. In Japan among almost one hundred national universities other than several hundred private universities, Ochanomizu and Nara are only for women students. This means that the level of the students is rather

high, which, however, does not mean a good place for a professor to perform active research. Namely HH had to struggle with no research assistant, no modern instruments, no fund, but with a few master and under-graduate students.

Luckily enough he called to remember his private research note on his first QSAR (quantitative structure-activity relationship) study, and with the knowledge of Hückel molecular orbital theory he could find his own graph-theoretical recipe for obtaining the coefficients of the characteristic polynomial, $P_G(x)=(-1)^N\det(\mathbf{A}-x\mathbf{E})$, for tree graph G by using the non-adjacent number, $p(G,k)$'s, as follows [4]:

$$P_G(x) = \sum_{k=0}^{\lfloor N/2 \rfloor} (-1)^k p(G,k) x^{N-2k} \quad (G \in \text{tree}). \tag{1}$$

Then the "topological index" Z is proposed to be defined as the sum of the $p(G,k)$'s as

$$Z = \sum_{k=0}^{\lfloor N/2 \rfloor} p(G,k). \tag{2}$$

The Z-counting polynomial $Q_G(x)$ is also defined as

$$Q_G(x) = \sum_{k=0}^{\lfloor N/2 \rfloor} p(G,k) x^k. \tag{3}$$

Naturally we have

$$Z = Q_G(1). \tag{4}$$

Many years later acyclic [5], reference [6], and matching [7] polynomials $M_G(x)$'s were proposed to be defined independently by several mathematical chemists and mathematicians, such as Zagreb group, Aihara, and Farrell.

$$M_G(x) = \sum_{k=0}^{\lfloor N/2 \rfloor} (-1)^k p(G,k) x^{N-2k}. \tag{5}$$

Since all of them are using the $p(G,k)$ numbers of HH, these polynomials are essentially the same as $Q_G(x)$.

Now let us go back to discuss our Z. HH succeeded in finding good correlation between several thermodynamic quantities, such as boiling point and entropy, and the Z obtained from the carbon atom skeleton graph of saturated hydrocarbon molecules.

In the autumn of 1970 HH read a paper on his TI at the Symposium on the Electronic Structure of Molecules held in Electro-Communication Univ. of Tokyo. Although his presentation of this new idea was welcomed by the audience at that time, HH had to be confronted by the conservative and hard wall of the societies of chemists all over the world.

First, the letter to Chemical Physics Letters was rejected severely from the following reasons. "Since such a simple proposal must have been made by some other people, try to explore document survey in

other fields of science. Further, physico-chemical discussion is lacking in this letter." In 1973 when HH met the Editor E. Heilbronner in Basel, he himself betrayed this secret and made his apology to HH.

Anyway the first paper of TI, "Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons" was published in Bulletin of the Chemical Society of Japan (BCSJ) in September of 1971 [4], but later HH was told that at least two designated referees quitted their job before this official debut of TI. They must have been severely vexed by the unique idea of *Z*-index.

However, after this a number of TI papers began to be proposed by chemists all over the world especially in Eastern Europe and US, and the term TI became a common noun. Thus *Z*-index of HH is now called as "the TI" or "Hosoya index," and according to Balaban HH is the "godfather" of TI [8]. Among many reviews and monographs introducing the TI's the book by Devillers and Balaban develops the detailed historical development of TI and *Z*-index [9], especially in the chapter by Ivanciuc and Balaban [10].

The first TI paper by HH [4] is now being cited frequently not only by mathematical chemists but also by mathematicians and information scientists. According to GoogleScholar the total citation number is exceeding 1700 as of the summer of 2018, and this number is increasing weekly nearly after half a century since its debut.

Notwithstanding of dramatic debut and checkered youth, things surrounding TI was changing into warm atmosphere especially after the turn of the century.

Ramon Carbo-Dorca, Professor of the Institute of Computational Chemistry, University of Girona organized Vth Girona Seminar on Molecular Similarity dedicated to HH. The invited guests were P. Mezey, J. Galvez, J. Devillers, E. Estrada, S. Basak, J. Cioslowski, S. Iwata, K. Hirao, and H. Nakatsuji, etc.

HH retired from Ochanomizu Univ. in the spring of 2002 after serving 31 years.[*1] He invited A. T. Balaban and M. Randic to Tokyo on this occasion, where Balaban declared that HH is the godfather of TI in his lecture at Ochanomizu [8]. As a matter of fact, most of the audience there didn't know the true meaning of "godfather" in Christianity but seemed to relate HH to the famous Mafia.

In September of 2002 the special issue in honor of HH was published in Inter-electronic J. of Molecular Design for which J.-I. Aihara was nominated as the guest editor [11]. On top of this issue Ref. [1] by HH is printed. Many distinguished mathematical chemists are contributing to it, such as A. T. Balaban, J. Gasteiger, N. F. Zefirov, N. Trinajstic, O. Ivanciuc, Y. Jiang, etc. All of the 50 contributed papers can freely be downloaded.

In October of 2002 International Symposium on Thirty-First Year of the Topological Index was

organized by U. Nagashima and K. Takano in Tokyo. Main Guests were: J-I Aihara, S. Fujita, A. Graovac, I. Gutman, S. Basak, and K. Funatsu.

§ 3 Topological index versus molecular descriptor

As introduced above the term "topological index" is a sloppy Japanese English invented by HH. Although there were proposed other names such as "molecular descriptor" by some groups of mathematical chemists [12,13], TI was gradually prevailing until now. The reason why HH is appreciating this big but invisible movement is as follows. If in the early stage such as in 1970's or 1980's the term molecular descriptor prevailed, almost no mathematicians got interested into such a fantastic world of TI, and as a result the new journal MATI would not be born out.

Although the Wiener index w is now known as the first TI, Wiener himself was concerned only with acyclic hydrocarbon molecules, or tree-graphs [2]. While his original definition of the path number w can be applied only to trees, HH redefined it by using the distance matrix **D**, which can commonly be applied to tree and non-tree graphs as in his first TI paper [4]. Due to this HH paper Wiener's w could gain such monumental position to date that is attracting the interest of many scientists including mathematicians.

The string of fate connecting HH and Wiener was still continuing up to 1988, when HH wrote a paper "On some counting polynomials in chemistry" in Discrete Applied Math. [14] where he proposed the following polynomial,

$$\mathrm{H}_{\mathrm{G}}(x) = \sum_{k=1}^{l} d_k x^k, \tag{6}$$

under the name of "Wiener polynomial," because the famous TI's of Wiener's w and p can formally be derived as follows.

$$w = \mathrm{H}'_G(1) \tag{7}$$

and

$$p = \mathrm{H}'''(0)/6. \tag{8}$$

However, thanks to I. Gutman et al. this polynomial (6) is now widely called as "Hosoya polynomial" [15]. They might have considered the contribution of HH who opened the Pandora's box.

Though not directly related to this topics, HH began to play with the "distance polynomial" $\mathrm{S}_{\mathrm{G}}(x)$ as early as 1973, when he proposed to define this polynomial by using the distance matrix **D** for a given graph as [16]

$$\mathrm{S}_{\mathrm{G}}(x) = (-1)^N \det(\mathbf{D} - x\mathbf{E}). \tag{9}$$

However, in a few years later Graham and Lovasz quite independently proposed to define the same polynomial [17]. These coincidental proposals triggered their joint work to yield a joint letter [18], which

was published in the very first issue of the J. Graph Theory edited by Frank Harary.

Although this was just a short letter of only three pages, it is one of the two monumental and important papers to HH that gave him the Erdös number of 2. Another one is a joint paper of HH and his academic uncle, Harary [19] on the perfect matching numbers of some interesting graphs, which, however, is not explained here.

§ 4 Various aspects of *Z*-index

In the beginning *Z*-index was found to have good correlation with several thermodynamic properties of saturated hydrocarbon molecules [4]. However, soon after that with a little modification it was shown to be well correlated also with the π-electronic energy *E*π of conjugated hydrocarbon molecules [20]. This property comes from the fact that *E*π of those molecules (either tree or non-tree) is determined from the zeros of the solution of $P_G(x)=0$. For trees $P_G(x)$ is closely related to *Z* through (1) and (2), whereas for non-trees we need such correction terms to (1) that are dependent on the degree of the ring structure. Thus in a global sense *Z*-index correlates roughly not only with various thermodynamic properties but also with π-electronic structure of molecules.

Now let us go back to more mathematical features about the *Z*-indices of various series of graphs. The *Z*-values of the path graphs S_n's are nothing else but the Fibonacci numbers, 1, 2, 3, 5, 8, ⋯, while those of the monocyclic rings C_n's starting from a triangle are the Lucas numbers, 4, 7, 11, 18, ⋯ [21]. These interesting properties are already introduced in the famous book by Koshy [22], together with the Hosoya triangle.

These interesting properties of *Z*-index are found to come from the close relationship between the two kinds of Chebyshev polynomials and the matching polynomials of path S_n and monocyclic ring graphs C_n. The second and first kinds of Chebyshev polynomials, U_n and T_n, are defined as follows [23]:

$$U_n(\cos\theta) = \sin(n+1)\theta / \sin\theta \tag{10}$$

and

$$T_n(\cos\theta) = \cos n\theta. \tag{11}$$

The matching polynomials of S_n and C_n graphs are obtained to be as given in Tables 1 and 2, respectively, which are compared to $U_n(x)$ and $T_n(x)$, respectively. Note the following equalities,

$$M_{Sn}(x) = U_n(x/2) \tag{12}$$

and

$$M_{Cn}(x) = 2\, T_n(x/2). \tag{13}$$

The sums of the absolute values of the coefficients of these two $M_G(x)$ polynomials are nothing else but the Fibonacci and Lucas numbers, respectively.

Table 1. S_n, U_n, and Fibonacci

S_n	$M_{Sn}(x) = U_n(x/2)$	$U_n(x)$	Z
ϕ	1	1	1
•	x	$2x$	1
	$x^2 - 1$	$4x^2 - 1$	2
	$x^3 - 2x$	$8x^3 - 4x$	3
	$x^4 - 3x^2 + 1$	$16x^4 - 12x^2 + 1$	5
	$x^5 - 4x^3 + 3x$	$32x^5 - 32x^3 + 6x$	8
	$x^6 - 5x^4 + 6x^2 - 1$	$64x^6 - 80x^4 + 24x^2 - 1$	13

Table 2. C_n, T_n, and Lucas

C_n	$M_{Cn}(x) = 2T_n(x/2)$	$T_n(x)$	Z
ϕ	2	1	2
•	x	x	1
	$x^2 - 2$	$2x^2 - 1$	3
	$x^3 - 3x$	$4x^3 - 3x$	4
	$x^4 - 4x^2 + 2$	$8x^4 - 8x^2 + 1$	7
	$x^5 - 5x^3 + 5x$	$16x^5 - 20x^3 + 5x$	11
	$x^6 - 6x^4 + 9x^2 - 2$	$32x^6 - 48x^4 + 18x^2 - 1$	18

There are two different types of Hermite polynomials as,

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \quad \text{(physicists')} \tag{14}$$

and

$$H_{e^n}(x) = (-1)^n e^{x^2/2} \frac{d^n}{dx^n} e^{-x^2/2} \quad \text{(probabilists')} \text{ [24].} \tag{15}$$

They are connected with each other as

$$H_{e^n}(x) = 2^{-n/2} H_n(x/\sqrt{2}). \tag{16}$$

According to Wolfram Mathworld, $H_{en}(x)$ is the independence (matching) polynomial of the complete graph K_n [25] as shown in Table 3. That is

$$M_{Kn}(x) = H_{en}(x). \tag{17}$$

Table 3. Complete graph K_n and Hermite polynomials.

n	K_n	$M_{Kn}(x) = H_{en}(x)$	$H_n(x)$	Z
0	ϕ	1	1	1
1	•	x	$2x$	1
2		$x^2 - 1$	$4x^2 - 2$	2
3		$x^3 - 3x$	$8x^3 - 12x$	4
4		$x^4 - 6x^2 + 3$	$16x^4 - 48x^2 + 12$	10
5		$x^5 - 10x^3 + 15x$	$32x^5 - 160x^3 + 120x$	26

In Table 3 are given the *Z*-values of K_n, which are found to be equal to the numbers of Young tableaux of size *n*, Y(n). Further, the *p*(G,*k*) numbers for K_n just correspond to the partial set of Y(*n*). For example see Fig. 1, where all the Young tableaux diagrams below *n*=5, are given together with the selection of non-adjacent edges for contributing to *p*(G,*k*) counting in red bars. The readers can realize this property by checking the coefficients of the *Z*-counting polynomial $Q_{Kn}(x)$, or $M_{Kn}(x)$, for a given set of *n* and *k*.

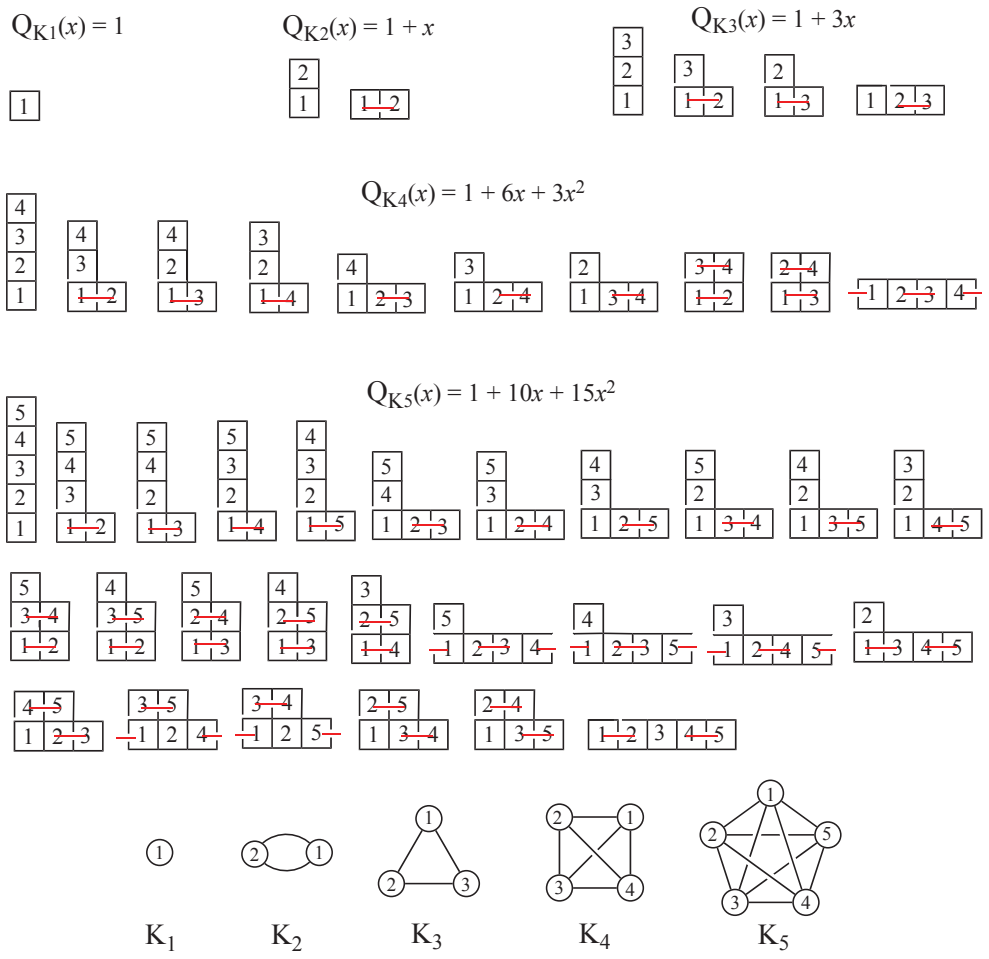

Fig. 1 Correlation between the *p*(G,*k*) selection for K_n and construction of Young tableaux diagrams.

In this way matching polynomials for typical series of graphs are found to be closely related to some of the orthogonal polynomials [26]. This means that the concept of the *p*(G,*k*) numbers and *Z*-index involves very important mathematical properties connecting between geometry and algebra. In this sense they are superior to other TI's.

On the other hand, from a global point of view *Z*-index can be proposed for using a rough sorting

device for coding and classifying the structures of various kinds of graphs [27].

Renowned computer scientist A. Mowshowitz wrote a paper “The Hosoya entropy of a graph” with M. Dehmer, an information scientist [28]. They got a hint from the *Z*-index of HH, and defined the partial Hosoya polynomial and further Hosoya entropy. Further many other Hosoya items are introduced by them, such as, Hosoya equivalent, Hosoya profile, Hosoya graph decomposition, etc. On the other hand, T. Aurues, a medical doctor in Japan, wrote an interesting paper “The Fibonacci sequences in nature implies thermodynamic maximum entropy” in which he writes that Z-index might provide the maximum entropy values of molecular surface electrons [29]. These two papers suggest that *Z*-index has some potential features related to entropy.

Thus, in spite of its debut in the QSAR study of chemical substances *Z*-index of HH was found to be applied not only to mathematical but also to a wide variety of scientific problems. Then in 2012 HH decided to write a monograph of TI but in Nihongo dedicated solely to its mathematical aspects intentionally excluding chemical relevance [30]. For the interested readers the chapter titles will be introduced here.

§ 1 The basic series of numbers and polynomials.

§ 2 Graph theory and TI.

§ 3 Non-tree graphs and their TI’s.

§ 4 Pell equation and TI.

§ 5 Indefinite equation of Diophantos and TI.

§ 6 Pythagorean triangles and TI.

§ 7 Further development of TI.

More extensive and dramatic development is expected for TI’s. This is the final remark from HH.

References

[1] H. Hosoya, *Internet Electronic J. Mol. Design*, **1** (2002) 428-442.

[2] H. Wiener, *J. Am. Chem. Soc*., **69** (1947) 17-20.

[3] J. R. Platt, *J. Phys. Chem*., **56** (1952) 328-336.

[4] H. Hosoya, *Bull. Chem. Soc. Jpn*., **44** (1971) 2332-2339.

[5] I. Gutman, M. Milun, N. Trinajstic, *Math. Chem.* (*Mülheim/Ruhr*), **1** (1975) 171-175.

[6] J.-I. Aihara, *J. Amer. Chem*. Soc., **98** (1976) 2750-2758.

[7] E. J. Farrell, *J. Comb. Theory*, **26B** (1979) 111-xxx; **27B** (1979) 75-86.

[8] A. T. Balaban, *J. Comput. Chem., Japan*, **16** (2017) 33-37.

[9] J. Devillers, A. T. Balaban (Eds.), Topological indices and related descriptors in QSAR and QSPR," Gordon Breach, Amsterdam (1999).

[10] O. Ivanciuc, A. T. Balaban, in Chpter 3 of Ref. [9].

[11] Special issue of *Interelectronic J. of Molecular Design*, **1** (2002), BioChem Press.

[12] L. B. Kier, L. H. Hall, Molecular connectivity in chemistry and drug research, Academic Press, New York (1976).

[13] M. Karelson, Molecular descriptors in QSAR/QSPR, Wiley, New York (2000).

[14] H. Hosoya, *Discrete Appl. Math*., **19** (1988) 239-257.

[15] I. Gutman, E. Estrada, O. Ivanciuc, Graph Theory Notes N. Y., **36** (1999) 7-13.

[16] H. Hosoya, M. Murakami, M. Gotoh, *Natl. Sci. Rept. Ochanomizu Univ*., **24** (1973) 27-34.

[17] R. L. Graham, L. Lovasz, *Adv. Math*., **29** (1978) 60-88.

[18] R. L. Graham, A. J. Hoffman, H. Hosoya, *J. Graph Theory*, **1** (1977) 85-88.

[19] H. Hosoya, F. Harary, *J. Math. Chem*., **12** (1993) 211-218.

[20] H. Hosoya, K. Hosoi, I. Gutman, *Theor. Chim. Acta*, **38** (1975) 37-47.

[21] H. Hosoya, *Fibonacci Quarterly*, **11** (1973) 255-266.

[22] T. Koshy, Fibonacci and Lucas numbers with applications, Wiley, New York (2001).

[23] Wikipedia, Chebyshev polynomials.

[24] Wikipedia, Hermite polynomial.

[25] WolframMathWorld, Hermite polynomial.

[26] H. Hosoya, *Natl. Sci. Rept. Ochanomizu Univ*., **32** (1981) 127-138.

[27] H. Hosoya, *J. Chem. Documentation*, **12** (1972) 181-183.

[28] A. Mowshowitz, M. Dehmer, *Entropy* (*Basel*), **17** (2015) 1054-1062.

[29] T. Aurues, *Kokyuroku of Res. Inst. Math. Sci. Kyoto Univ.*, **1852** (2013) 165-176.

[30] H. Hosoya, Topological index—New mathematics bridging from Fibonacci numbers to Pythagorean triangles—, (in Nihongo), Nihon-Hyoronsha, Tokyo (2012).

*1 $1936=44^2$. HH is declaring "I will survive at least until $2025=45^2$."

*2 HH retired Ochanomizu in 2002 after serving 31 years. Behold that $2002=2\times7\times11\times13$ and $2+7+11+13=31$.