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Formulas for the Hyper-Wiener and Hyper-Detour Indices of Fused Bicyclic Structures

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Abstract

It was shown that the hyper-detour and hyper-Wiener indices are fourth order polynomials in terms of the sizes of strings. The respective formulas were derived for all subcases.

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Introduction

The detour index[1] Γ and the hyper detour index[2] γ are analogues of the well known Wiener[3] Ω and hyper -Wiener indices[4] ω, respectively. Ω is the sum of distances between all pairs of atoms (vertices) in a hydrogen suppressed graph (hydrogen suppressed graphs will be considered in this paper, only).

$$\Omega = \Sigma\, D_{\alpha\beta} \tag{1}$$

where $D_{\alpha\beta}$ denotes the length of the shortest path between vertices α, β and the summation has to be performed for all pairs of vertices. The detour index Γ may be obtained by replacing $D_{\alpha\beta}$ by $\Delta_{\alpha\beta}$ in Eq. (1) where $\Delta_{\alpha\beta}$ denotes the

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length of the longest path between vertices α, β. The Wiener and the detour indices are equivalent in acyclic systems, but are different in cycle containing structures.

The hyper Wiener index ω was proposed by Randic[4]. However, the algorithm suggested by Randic could be applied for acyclic structures alone. It was shown[5] that ω is equal to

$$\omega = \Sigma(D_{\alpha\beta} + D_{\alpha\beta}{}^2)/2 \qquad (2)$$

and that this formula may also be used to extend the definition of ω to cycle-containing structures. The hyper-detour index[2] γ is an analogue of ω, where $D_{\alpha\beta}$ must be replaced by $\Delta_{\alpha\beta}$, in Eq. (2). From the above definitions it is clear that $\Omega < \Gamma$ and $\omega < \gamma$ in cycle-containing structures, and also $\Omega < \omega$ and $\Gamma < \gamma$ in all structures - but methane and ethane. The following example illustrates the computation of Ω, Γ, ω and γ. Let us consider the hydrogen suppressed graph of cyclobutane (Fig. 1). The distances and the length of the detour paths are as follows. $D_{12} = 1$, $D_{13} = 1$, $D_{14} = 2$, $D_{23} = 2$, $D_{24} = 1$, $D_{34} = 1$; $\Delta_{12} = 3$, $\Delta_{13} = 3$, $\Delta_{14} = 2$, $\Delta_{23} = 2$, $\Delta_{24} = 3$, $\Delta_{34} = 3$. The respective values of the indices are: $\Omega = 8$, $\Gamma = 16$, $\omega = 10$, $\gamma = 30$. It has to be noted that the Rouvray index[6] is equal to 2Ω.

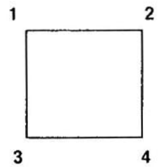

Fig. 1: Hydrogen suppressed graph of cyclobutane.

The Wiener index is one of the most popular graph theoretical invariants that was applied many times in chemistry. The reader may find several reviews on various aspects concerning its properties and uses[7,8,9]. Many new topological indices, also closely related to the Wiener index, were suggested by Diudea[10] recently.

Ω and ω may be calculated by using one of the numerous methods to obtain the distances. On the other hand it is not possible to construct the detour matrix in an efficient way, although an algorithm[11] is now available to compute values of $\Delta_{\alpha\beta}$. Besides numerical methods, formulas may also be used to calculate values of Ω and ω for various types of structures. Formulas may be used to solve the famous "graph reconstruction problem" - i.e. to find a graph which corresponds to a definite value of an index - at least for those kinds of graphs for which the formulas are known.

It was shown[12,13] that Ω is a third order and ω is a fourth order polynomial in terms of the sizes of strings (see definition in the next section) making up a graph. It was also shown that Γ is a third order polynomial in terms of the sizes of strings if the underlying graph is a cutpoint graph consisting of simple cycles and acyclic branches[5]. Furthermore it was shown[11] that the complete graph containing ζ vertices has the highest value of Γ of all graphs containing ζ vertices and that Γ is a third order polynomial in terms of ζ. This result means that once for a given type of graphs Γ may be calculated by using a polynomial in terms of the sizes of the strings, then the order of this polynomial can not be higher than three.

The aim of the present paper was to show that such polynomials can be constructed for fused bicyclic graphs (FBG's). FBG's are the simplest graphs which are not cutpoint graphs. The results will be extended to the hyper-detour index and it will be shown that γ is a fourth order polynomial in FBG's. Since $\omega < \gamma$, the order of a polynomial of the hyper-Wiener index can also not be higher than four. Formulas were derived that allow to compute ω and γ for FBG's.

A Theorem

Expressions denoting basically the same concepts in chemistry and graph theory like "structural formula" and "graph", "atom" and "vertex", "chemical bond", and "edge", "valence" and "degree" will be used interchangeably hereafter. An "endpoint" denotes a vertex the valence of which is one. Alternatively a "branching vertex" denotes a vertex the valence of which is higher than two. A "chain" consists of two endpoints and the degree of the other vertices (if there are any) is equal to two. A "string" is a chainlike subgraph that starts with a branching vertex or an endpoint, and ends with a branching vertex or an endpoint. The "size" of a string denotes the number of vertices in the string. Examples: n-butane consists of a single string, the size of which is four. Isobutane consists of three strings, the size of each is equal to two. The branching atom belongs to three strings simultaneously. The structure depicted in Fig. 2 is an FBG which consists of three strings k, m and n. The sizes are 12, 10 and 5, respectively. Note that the strings and their sizes will be denoted by the same letter. The total number of atoms is equal to $\zeta = k + m + n - 4$ in FBG's. It will be shown that the hyper-Wiener and the hyper-detour indices of FBG's are polynomials in terms of the sizes of the strings. For the sake of simplicity the proof will be given for the detour index showing that Γ is a polynomial in terms of the sizes of strings. The same arguments can then be used to show that γ is a polynomial, too. Because of a theorem proved earlier[11], the order of that polynomial can not be higher than four.

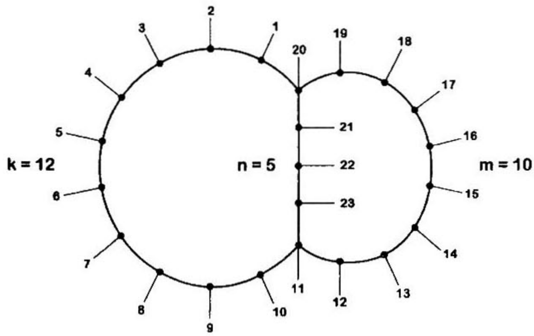

Fig. 2: A general scheme of a fused bicyclic graph (Bicyclo[10.8.3]trieicosan which is used as an example)

Fig. 2 is illustrates the domains for which the expressions given in Tab. 1 were derived. The numbering of the vertices starts at the second vertex in string k. The (k-1)-th vertex belongs to strings k and m and n. Vertex $k + m - 2$ also belongs the these strings simultaneously. All paths starting at vertex α and ending at vertex β ($\alpha < \beta$) will be considered. Each path may be grouped into one of the six cases (Tab. 1) depending on the position where the path starts and where it ends. Tab. 1 lists the various cases and the length of the longest path in FBG's. In cases 3a, 3b and 6 only one portion of the string will be considered because of symmetry reasons. The direction of the longest route is also shown in the last column of Tab. 1. Here we use the following convention: k, m and n denote a walk in the direction of increasing numbers, whereas -k, -m and -n denote walks in the opposite direction.

Table 1. Expressions defining the longest path in FBG's

Case	from	to	$\Delta_{\alpha\beta}$	Route
1a	k	k	$\beta-\alpha$	k
1b	k	k	$\alpha-\beta+k+m-2$	-k-m-k
2	m	m	$\alpha-\beta+k+m-2$	-m-k-m
3a	k *	m	$\beta-\alpha$ **	km
3b	k *	m	$2k-m-n-\beta-\alpha$	k-n-m
4	k *	n	$\beta-\alpha$	kmn
5	n	n	$\alpha-\beta+k+n-2$	-nk-n
6	m **	n	$3k+2m+n-6-\beta-\alpha$	mk-n

* $1 \le \alpha \le \left[\frac{k-1}{2}\right]$, ** $k \le \alpha \le k-1+\left[\frac{m-1}{2}\right]$

Cases 1a, 1b, 2, 3a and 3b: the longest path and the shortest path between α and β together form a cycle, the size of which is $k + m - 2$ and for this cycle Γ is a third order polynomial[5] and γ is a fourth order polynomial in terms of k and m. In case 3b the longest path does not lie on this cycle, the difference is $2k + m + n - 4 - i - j - (j - i) = 2k + m + n - 4 - 2j$. In this way all pairs of vertices of cycle $k + m$ are accounted for and we have third (fourth) order polynomial plus the sum of the "correction terms" related to case 3b. The sum for the respective values of α and β will yield a third (fourth) order polynomial in terms of k, m and n for the "correction term", too.

Case 4: The starting atoms α lie on a string beginning with 1 and ending with vertex $[(k-1)/2]$, where [and] are the Gaussian brackets (i.e. [r] is the greatest integer not exceeding the real number r). The target vertices β lie in on a string beginning with vertex k + m - 1 and ending at vertex k + m + n - 4 and we can replace the FBG with a chain of size k + m + n - 4. The sum of the lengths of the paths is clearly a third (fourth) order polynomial in terms of k, m and n. Case 6: The length of the equivalent chain is again k + m + n - 4. Therefore the same arguments used for Case 4 may also be applied for this case.

Case 5: Both α and β are located on string n. The longest path connecting α and β includes strings k and n. Therefore the sum of all detour paths is a fraction of the detour (hyper-detour) index related to the cycle k + n, which is a third (fourth) order polynomial[2] in terms of k and n.

We can now state our theorem: in FBG's Γ is a third and γ is a fourth order polynomial in terms of the sizes of strings. Note that the present proof is a constructive one, meaning that it could be used to derive these polynomials. We shall apply another technique in the next section to derive the formulas for ω and γ.

Numerical Method

The formulas of the hyper-Wiener and hyper-detour indices will be sought in the following form:

$$\Lambda = Ak^4 + Bm^4 + Cn^4 + Dk^3m + Ek^3n + Fkm^3 + Gkn^3 + Hm^3n + Imn^3 + Jk^2m^2 + Kk^2n^2 + Lm^2n^2 + Mk^2mn + Nkm^2n + Okmn^2 + Pk^3 + Qm^3 + Rn^3 + Sk^2m + Tkm^2 + Uk^2n + Vkn^2 + Wm^2n + Xmn^2 + Ykmn + ak^2 + bm^2 + cn^2 + dkm + ekn + fmn + gk + hm + in + j; \quad \Lambda = (\gamma, \omega) \qquad (3)$$

where coefficients A, B, ..., Y, a, b,...,j have to be determined. There are 35 unknowns altogether, meaning that 35 known cases (i.e. for which the values of the terms $k^x m^y n^z$ are known, where $x + y + z = 0, 1, 2, 3, 4$). The coefficients may be obtained by solving a system of 35 linear equations.

In simple cycles the formulas of γ and ω depend on the parity of ζ, two slightly differing formulas exist for ζ = even number and for ζ = odd number[4,5]. Because of this fact there are four cases ($k \leq m \leq n$)

Case I: k, m and n are even, or k, m, n are odd.

Case II: k and m are odd n is even, or k and m are even and n is odd

Case III: k is even and m and n are odd, or k is odd m and n are even.

Case IV: k and n are even and m is odd, or k and n are odd and m is even This would mean that we need 4x35 = 140 different examples to obtain the formulas for γ (or ω). This task could be simplified since the coefficients A, B, ... Y related to the third and fourth order terms must be equal in all cases, only coefficients a, b,...,j related to the second , first and zero order terms may vary. There are ten "lowercase" coefficients, and once the "uppercase" coefficients are known, ten equations are needed for cases II, III and IV, each. The equations can not depend on the choice of numbers k, m and n, however, it may happen very often, that the matrix composed of terms $k^x m^y n^z$ (x+y+z = 0,1,2,3,4) is singular. Tab. 2 lists a set of strings for which this matrix is not singular.

Table 2. Structures with a Non-singular Matrix of Polynomials (Case 1).

k	m	n	ω	γ	k	m	n	ω	γ
2	2	2	1	1	16	6	6	5525	43855
4	2	2	10	30	12	10	6	4890	45699
6	4	2	101	600	5	5	5	265	1819
4	4	2	37	186	7	5	5	495	3719
6	2	2	42	168	9	7	3	902	7387
12	4	2	825	5600	9	9	3	1419	12365
8	6	6	1045	8535	7	7	5	830	6720
10	4	4	745	5080	9	5	3	555	4032
10	6	2	740	5840	7	3	3	153	860
8	6	2	415	3166	11	9	3	2159	19413
6	4	4	197	1298	11	5	3	973	7141
6	6	4	375	2781	9	7	5	1346	11336
8	6	4	674	5283	5	5	3	139	897
8	8	2	713	5954	7	7	3	528	4121
10	8	6	2428	21523	9	7	7	1960	16960
8	4	4	402	2734	11	11	3	3118	29237
6	6	6	630	4830	13	5	3	1599	11759
8	8	4	1097	9185					

Results and Discussion

The derived equations are listed below:

Case I: (k, m and n are even, or k, m, n are odd)

$$\gamma = (7k^4 + 5m^4 + 5n^4 + 28k^3m + 14k^3n + 32km^3 + 32kn^3 + 14m^3n + 16mn^3 + 51k^2m^2 + 39k^2n^2 + 27m^2n^2 + 78k^2mn + 78km^2n + 72kmn^2 - 87k^3 - 85m^3 - 104n^3 - 351k^2m - 357km^2 - 252k^2n - 324kn^2 - 240m^2n - 264mn^2 - 588kmn + 524k^2 + 556m^2 + 586n^2 + 1272km + 1088kn + 1044mn - 1356k - 1388m - 1324n + 1152)/48 \qquad (4)$$

$$\omega = (1k^4 + 1m^4 + 3n^4 + 2k^3m + 4k^3n + 2km^3 + 2kn^3 + 4m^3n + 2mn^3 + 3k^2m^2 + 3k^2n^2 + 3m^2n^2 + 6k^2mn + 6km^2n + 0kmn^2 - 9k^3 - 9m^3 - 6n^3 - 12k^2m - 12km^2 - 21k^2n - 15kn^2 - 21m^2n - 15mn^2 - 12kmn + 20k^2 + 20m^2 + 18n^2 + 20km + 24kn + 24mn - 12k - 12m - 12n + 0)/48 \qquad (5)$$

Case II: (k and m are odd, n is even, or k and m are even and n is odd)

$$\gamma = (7k^4 + 5m^4 + 5n^4 + 28k^3m + 14k^3n + 32km^3 + 32kn^3 + 14m^3n + 16mn^3 + 51k^2m^2 + 39k^2n^2 + 27m^2n^2 + 78k^2mn + 78km^2n + 72kmn^2 - 87k^3 - 85m^3 - 104n^3 - 351k^2m - 357km^2 - 252k^2n - 324kn^2 - 240m^2n - 264mn^2 - 588kmn + 533k^2 + 565m^2 + 580n^2 + 1284km + 1100kn + 1056mn - 1428k - 1460m - 1360n + 1263)/48 \qquad (6)$$

$$\omega = (1k^4 + 1m^4 + 3n^4 + 2k^3m + 4k^3n + 2km^3 + 2kn^3 + 4m^3n + 2mn^3 + 3k^2m^2 + 3k^2n^2 + 3m^2n^2 + 6k^2mn + 6km^2n + 0kmn^2 - 9k^3 - 9m^3 - 6n^3 - 12k^2m - 12km^2 - 21k^2n - 15kn^2 - 21m^2n - 15mn^2 - 12kmn + 14k^2 + 14m^2 + 18n^2 + 8km + 24kn + 24mn + 9k + 9m + 6n - 21)/48 \qquad (7)$$

<u>Case III:</u> (k is even and m and n are odd, or k is odd m and n are even)

$$\gamma = (7k^4 + 5m^4 + 5n^4 + 28k^3m + 14k^3n + 32km^3 + 32kn^3 + 14m^3n + 16mn^3 + 51k^2m^2 + 39k^2n^2 + 27m^2n^2 + 78k^2mn + 78km^2n + 72kmn^2 - 87k^3 - 85m^3 - 104n^3 - 351k^2m - 357km^2 - 252k^2n - 324kn^2 - 240m^2n - 264mn^2 - 588kmn + 527k^2 + 562m^2 + 595n^2 + 1278km + 1094kn + 1062mn - 1377k - 1439m - 1372n + 1218)/48 \quad (8)$$

$$\omega = (1k^4 + 1m^4 + 3n^4 + 2k^3m + 4k^3n + 2km^3 + 2kn^3 + 4m^3n + 2mn^3 + 3k^2m^2 + 3k^2n^2 + 3m^2n^2 + 6k^2mn + 6km^2n + 0kmn^2 - 9k^3 - 9m^3 - 6n^3 - 12k^2m - 12km^2 - 21k^2n - 15kn^2 - 21m^2n - 15mn^2 - 12kmn + 17k^2 + 17m^2 + 18n^2 + 14km + 18kn + 18mn + 9k + 0m + 3n - 18)/48 \quad (9)$$

<u>Case IV:</u> (k and n are even and m is odd, or k and n are odd and m is even)

$$\gamma = (7k^4 + 5m^4 + 5n^4 + 28k^3m + 14k^3n + 32km^3 + 32kn^3 + 14m^3n + 16mn^3 + 51k^2m^2 + 39k^2n^2 + 27m^2n^2 + 78k^2mn + 78km^2n + 72kmn^2 - 87k^3 - 85m^3 - 104n^3 - 351k^2m - 357km^2 - 252k^2n - 324kn^2 - 240m^2n - 264mn^2 - 588kmn + 536k^2 + 553m^2 + 595n^2 + 1278km + 1106kn + 1050mn - 1413k - 1403m - 1372n + 1218)/48 \quad (10)$$

$$\omega = (1k^4 + 1m^4 + 3n^4 + 2k^3m + 4k^3n + 2km^3 + 2kn^3 + 4m^3n + 2mn^3 + 3k^2m^2 + 3k^2n^2 + 3m^2n^2 + 6k^2mn + 6km^2n + 0kmn^2 - 9k^3 - 9m^3 - 6n^3 - 12k^2m - 12km^2 - 21k^2n - 15kn^2 - 21m^2n - 15mn^2 - 12kmn + 17k^2 + 17m^2 + 18n^2 + 14km + 18kn + 18mn - 0k - 9m - 3n - 18)/48 \quad (11)$$

The derived formulas can be used together with those derived earlier to find strings which would produce a given value of the hyper-Wiener or the hyper-detour indices. In this way a partial numerical solution of the "graph reconstruction problem" [14,15] may be obtained.

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