MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **90** (2023) 235–245
ISSN: 0340–6253
doi: 10.46793/match.90-1.235Y

Further Variants of Gutman's Formulas

Luzhen Ye

School of Science, Jimei University, Xiamen 361021, China

lzye555@sina.com

(Received January 7, 2023)

Abstract

Let $G = (U, V)$ be a connected bipartite graph and let $C(G)$ be the algebraic structure count of G. Gutman's formulas in [12] states that for any edge ab of G, then there exists an $\varepsilon \in \{1, -1\}$ such that

$$C(G) = |c(G - ab) + \varepsilon C(G - a - b)|.$$

The current author extended the above result and obtained some variants of Gutman's formulas in [21, 22] as follows.

1. For any $a, c \in U, b, d \in V$, then there exists an $\varepsilon_1 \in \{1, -1\}$ such that

$$C(G)C(G - a - b - c - d) = \\ |C(G - a - b)C(G - c - d) + \varepsilon_1 C(G - a - d)C(G - b - c)|.$$

2. For any 2-matching $\{u_1v_1, u_2v_2\}$ of G, then there exists an $\varepsilon_2 \in \{1, -1\}$ such that

$$C(G)C(G - u_1v_1 - u_2v_2) = \\ |C(G - u_1v_1)C(G - u_2v_2) + \varepsilon_2 C(G - u_1 - v_2)C(G - u_2 - v_1)|,$$

where $u_1, u_2 \in U, v_1, v_2 \in V$.

3. For any edge yz and two vertices r and s of G satisfying $y, r \in U$ and $z, s \in V$ and $\{y, z\} \cap \{r, s\} = \emptyset$, then there exists an $\varepsilon_3 \in \{1, -1\}$ such that

$$C(G)C(G - yz - r - s) = \\ |C(G - yz)C(G - r - s) + \varepsilon_3 C(G - y - s)C(G - r - z)|.$$

In this note, we prove that, if $|U| = |V| = n$, then there exists a $\beta = (\nu_1, \nu_2, \ldots, \nu_m)$ satisfying $\nu_1, \nu_2, \ldots, \nu_m \in \{1, -1\}$ such that

$$(m - n)C(G) = \left| \sum_{i=1}^{m} \nu_i C(G - e_i) \right|,$$

where the sum ranges over all edges $e_1, e_2, \ldots, e_m$ of G.

1 Introduction

Assume that G is a connected bipartite graph and (U, V) is its bipartition. Let $U = \{u_1, u_2, \ldots, u_{n_1}\}, V = \{v_1, v_2, \ldots, v_{n_2}\}$. The bipartite adjacency matrix of G is an $n_1 \times n_2$ matrix $B(G) = (b_{ij})$ satisfying

$$b_{ij} = \begin{cases} 1 & \text{if } u_i v_j \text{ is an edge of } G, \\ 0 & \text{otherwise.} \end{cases}$$

Hence the adjacency matrix of G can be expressed by

$$A(G) = \begin{pmatrix} 0 & B(G) \\ B(G)^T & 0 \end{pmatrix}.$$

Obviously, if $n_1 \neq n_2$, then $\det(A(G)) = 0$, and if $n_1 = n_2 = n$, then

$$\det(A(G)) = (-1)^n \det(B(G))^2. \tag{1}$$

Note that if $n_1 = n_2 = n$, i.e., $|U| = |V| = n$, then each nonzero term $sgn(\alpha) b_{1\alpha(1)} b_{2\alpha(2)} \ldots b_{n\alpha(n)}$ in the expansion of the determinant $\det(B(G))$ of $B(G)$ equals 1 or -1, where $\alpha(1)\alpha(2)\ldots\alpha(n)$ is a permutation of $1, 2, \ldots, n$. Furthermore, $sgn(\alpha) b_{1\alpha(1)} b_{2\alpha(2)} \ldots b_{n\alpha(n)} = 1$ or -1 if and only if $\{u_i v_{\alpha(i)} | 1 \leq i \leq n\}$ is a perfect matching of G. If $sgn(\alpha) b_{1\alpha(1)} b_{2\alpha(2)} \ldots b_{n\alpha(n)} = 1$, then we call $M_\alpha = \{u_i v_{\alpha(i)} | 1 \leq i \leq n\}$ to be an "even" perfect matching of G, and if $sgn(\alpha) b_{1\alpha(1)} b_{2\alpha(2)} \ldots b_{n\alpha(n)} = -1$, we call $M_\alpha = \{u_i v_{\alpha(i)} | 1 \leq i \leq n\}$ to be an "odd" perfect matching of G. Let $\mathcal{E}(G)$ and $\mathcal{O}(G)$ be the set of "even" and "odd" perfect matchings of G, respectively. Hence

$$\det(B(G)) = |\mathcal{E}(G)| - |\mathcal{O}(G)|. \tag{2}$$

Moreover, if we use $M(G)$ to denote the number of perfect matchings of G, then

$$M(G) = |\mathcal{E}(G)| + |\mathcal{O}(G)|. \tag{3}$$

Wilcox, a theoretical organic chemist, defined the algebraic structure count of a bipartite graph $G = (U, V)$ in [18, 19], denoted by $C(G)$, as the difference between the number of "even" and "odd" perfect matchings of G if $|U| = |V|$, and $C(G) = 0$ if $|U| \neq V$. Hence, if $|U| = |V|$,

$$C(G) = ||\mathcal{E}(G)| - |\mathcal{O}(G)|| = |\det(B(G))|. \tag{4}$$

By Eq. (1),

$$\det(A(G)) = (-1)^n C(G)^2. \tag{5}$$

A cycle C_k of G with k vertices is a nice cycle if $G - C_k$ has perfect matchings. It is well known [8, 9] that if each nice cycle C_k in G satisfies $k = 2$ (mod 4), then

$$C(G) = M(G). \tag{6}$$

i.e., the algebraic structure count of G equals the number of perfect matchings of G, which implies that all perfect matchings of G are "ever" (or "odd").

The relation between $C(G)$ and $M(G)$ has been studied extensively [7, 11, 14]. For example, if the number k of edges in each interior face in a plane bipartite graph G satisfies $k = 2$ (mod 4), then Eq. (6) holds [6]. In particular, all hexagonal systems G, the molecular graphs of benzenoid hydrocarbons, satisfy Eq. (6).

On the other hand, $C(G)$ has a closed relation with the thermodynamic stability of the corresponding molecular graphs and has important applications in theoretical organic chemistry [10, 13, 14, 17, 20]. On the further research on $C(G)$, see references [1, 2, 4, 5, 12, 15, 21].

For any edge $e = xy$ and any perfect matching M of G, either $e \in M$ or $e \notin M$. Hence

$$M(G) = M(G - x - y) + M(G - e), \tag{7}$$

where $G-x-y$ (or $G-e$) is the graph obtained from G by deleting vertices x and y (or e).

Gutman [12] obtained a similar result to Eq. (7) on the algebraic structure count of a bipartite graph G , and proved that for any any edge

$e = xy$ of G, one of the following relations holds.

$$C(G) = C(G-e) + C(G-x-y), \tag{8}$$

$$C(G) = C(G-e) - C(G-x-y), \tag{9}$$

$$C(G) = C(G-x-y) - C(G-e). \tag{10}$$

Gutman's formulas above show that there exists an $\varepsilon \in \{1, -1\}$ such that

$$C(G) = |C(G-e) + \varepsilon C(G-x-y)|. \tag{11}$$

Motivated by Eqs. (8)-(10), the current author obtained some variants of Gutman's formulas above in [21, 22] as follows.

Let $G = (U, V)$ be a bipartite graph. Then

1. For any $a, c \in U, b, d \in V$, then there exists an $\varepsilon_1 \in \{1, -1\}$ such that

$$C(G)C(G-a-b-c-d) = |C(G-a-b)C(G-c-d) + \varepsilon_1 C(G-a-d)C(G-b-c)|. \tag{12}$$

2. For any 2-matching $\{f = u_1v_1, g = u_2v_2\}$ of G, then there exists an $\varepsilon_2 \in \{1, -1\}$ such that

$$C(G)C(G-f-g) = |C(G-f)C(G-g) + \varepsilon_2 C(G-u_1-v_2)C(G-u_2-v_1)|, \tag{13}$$

where $u_1, u_2 \in U, v_1, v_2 \in V$.

3. For any edge $h = yz$ and two vertices r and s of G satisfying $y, r \in U$ and $z, s \in V$ and $\{y, z\} \cap \{r, s\} = \emptyset$, then there exists an $\varepsilon_3 \in \{1, -1\}$ such that

$$C(G)C(G-h-r-s) = |C(G-h)C(G-r-s) + \varepsilon_3 C(G-y-s)C(G-r-z)|. \tag{14}$$

Further to the above results, i.e., Eqs.(11)-(14), in this note, we continue to find the new variants of Gutman's formulas. We obtain a formula on $C(G)$ and all $C(G-e_1), C(G-e_2), \ldots, C(G-e_m)$ for any bipartite graph G with edge set $\{e_1, e_2, \ldots, e_m\}$.

2 The main result

In this section, we prove mainly the following result.

Theorem 1. *Let G be a connected bipartite graph with bipartition (U, V). If $|U| = |V| = n$, then there exists a $\beta = (\nu_1, \nu_2, \ldots, \nu_m)$ satisfying $\nu_1, \nu_2, \ldots, \nu_m \in \{1, -1\}$ such that*

$$(m-n)C(G) = \left| \sum_{i=1}^{m} \nu_i C(G - e_i) \right|, \tag{15}$$

where the sum ranges over all edges $e_1, e_2, \ldots, e_m$ of G. Particularly, if $C(G) = M(G)$, then

$$(m-n)C(G) = \sum_{i=1}^{m} C(G - e_i). \tag{16}$$

Proof. Let $B(G), B(G - e_1), B(G - e_2), \ldots, B(G - e_m)$ be the bipartite adjacency matrices of $G, G - e_1, G - e_2, \ldots, G - e_m$, respectively. For convenience, for $i = 1, 2, \ldots, m$, set

$$B = B(G) = (b_{st})_{n \times n}, B_i = B(G - e_i) = (b_{st}^{(i)}),$$

and let $\mathcal{S}_n$ be the symmetric group of oder n.

If G has no perfect matching, then $G - e_i$ has no perfect matching for $i = 1, 2, \ldots, m$. Hence $C(G) = C(G - e_1) = C(G_2) = \ldots = C(G - e_m) = 0$. Obviously, the theorem holds. Hence we may assume that G (resp. $G - e_i$) has $p + q$ (resp. $p_i + q_i$) perfect matchings, where p (resp. p_i) perfect matchings are "even", and q (resp. q_i) perfect matchings are "odd". Hence, by Eqs. (2) and (4), we have

$$\det(B) = p - q, \ \det(B_i) = p_i - q_i, \tag{17}$$

and

$$C(G) = |p - q|, \ C(G - e_i) = |p_i - q_i|, \tag{18}$$

for $i = 1, 2, \ldots, m$.

Denote the set of perfect matchings of G by $\{M_k|1 \leq i \leq p+q\}$, where $M_k = \{u_i v_{\alpha_k(i)}|1 \leq i \leq n\}$ and $\alpha_k \in \mathcal{S}_n$. Without loss of generality, we assume that the set of "even" perfect matchings of G is $\{M_1, M_2, \ldots, M_p\}$ and the set of "odd" perfect matchings of G is $\{M_{p+1}, M_{p+2}, \ldots, M_{p+q}\}$. Hence in the expansion of the determinant of B, all non-zero terms satisfy:

$$sgn(\alpha) b_{1\alpha_k(1)} b_{2\alpha_k(2)} \ldots b_{n\alpha_k(n)} = \begin{cases} 1, & \text{if } 1 \leq k \leq p, \\ -1, & \text{if } p+1 \leq k \leq p+q. \end{cases}$$

Let $\mathcal{L} = (l_{st})$ be a $(p+q) \times m$ matrix defined as

$$l_{st} = \begin{cases} 1, & \text{if } 1 \leq s \leq p \text{ and } e_t \notin M_s, \\ -1, & \text{if } p+1 \leq s \leq p+q \text{ and } e_t \notin M_s, \\ 0, & \text{otherwise.} \end{cases}$$

Since each perfect matching M_s of G contains exactly n edges, there $m-n$ edges in G each of which is not in M_s. Hence

$$r_s = \sum_{t=1}^{m} l_{st} = \begin{cases} m-n, & \text{if } 1 \leq s \leq p, \\ -(m-n), & \text{if } p+1 \leq s \leq p+q. \end{cases}$$

So

$$\sum_{s=1}^{p+q} \sum_{t=1}^{m} l_{st} = r_1 + r_2 + \ldots + r_{p+q} = (m-n)(p-q). \tag{19}$$

On the other hand, note that, for any $1 \leq i \leq m$, each non-zero term in the expansion of $\det(B_i)$ must be some non-zero term in the expansion of $\det(B)$, which is equal to 1 or -1. Particularly, they have the same sign. It is not difficult to see that we have

$$c_t = \sum_{s=1}^{p+q} l_{st} = p_t - q_t, \text{ for } 1 \leq t \leq m. \tag{20}$$

Thus

$$\sum_{s=1}^{p+q} \sum_{t=1}^{m} l_{st} = \sum_{t=1}^{m} \sum_{s=1}^{p+q} l_{st} = \sum_{t=1}^{m} c_t = \sum_{t=1}^{m} (p_t - q_t). \tag{21}$$

By Eqs. (19) and (21),

$$(m-n)(p-q)=\sum_{i=1}^{m}(p_i-q_i). \tag{22}$$

Then the following formula is immediate from Eq. (18).

$$|m-n|C(G)=\left|\sum_{i=1}^{m}(p_i-q_i)\right|. \tag{23}$$

Note that G is a connected bipartite graph with $2n$ vertices. So $m>n$ ($m\geq 2n-1$). Then there exists a $\beta=(\nu_1,\nu_2,\ldots,\nu_m)$ satisfying $\nu_1,\nu_2,\ldots,\nu_m\in\{1,-1\}$ such that

$$(m-n)C(G)=\left|\sum_{i=1}^{m}\nu_i|p_i-q_i|\right|=\left|\sum_{i=1}^{m}\nu_i C(G-e_i)\right|. \tag{24}$$

Hence we have proved that Eq. (15) holds.

Particularly, if $M(G)=C(G)$, then $p=0$ or $q=0$, which results in $p_i=0$ or $q_i=0$ for $1\leq i\leq m$. Then Eq. (16) follows from Eq. (22).

The theorem has been proved. ■

From the proof of the theorem above, the following results are immediate.

Corollary. *Let G be a connected bipartite graph with $2n$ vertices and m edges $e_1,e_2,\ldots,e_m$. Then*

$$(m-n)C(G)\leq\sum_{i=1}^{m}C(G-e_i). \tag{25}$$

Corollary. *Let G be a bipartite graph with $2n$ vertices and m edges $e_1,e_2,\ldots,e_m$. If each nice cycle C_k in G satisfies $k=2$ (mod 4), then*

$$(m-n)C(G)=\sum_{i=1}^{m}C(G-e_i). \tag{26}$$

A direct corollary of the theorem above is the following, which was ever found by Farrell and Wahid [3] and Wahid [16].

Corollary. *Let G be a connected bipartite graph with $2n$ vertices and m edges $e_1, e_2, \ldots, e_m$. Then the number of perfect matchings of G satisfies:*

$$(m-n)M(G) = \sum_{i=1}^{m} M(G-e_i). \tag{27}$$

Proof. In the proof of Theorem 1, if we set $\mathcal{L}' = (l'_{st})$ be a $(p+q) \times m$ matrix defined as

$$l'_{st} = \begin{cases} 1, & \text{if } e_t \notin M_s, 1 \leq s \leq p+q, \\ 0, & \text{otherwise.} \end{cases}$$

Similarly, we can prove that

$$(m-n)(p+q) = \sum_{i=1}^{m} (p_i + q_i) \tag{28}$$

which implies that Eq. (26) holds. ■

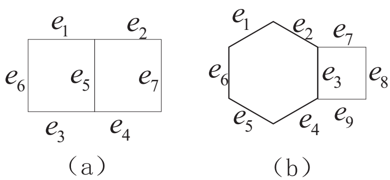

Figure 1. (a). A bipartite graph G_1. (b). A bipartite graph G_2.

3 Discussion

In this note, we use a combinatorial technique to obtain a formula on the algebraic structure counts $C(G), C(G-e_1), C(G-e_2), \ldots, C(G-e_m)$ for any bipartite graph G with $2n$ vertices and edge set $\{e_1, e_2, \ldots, e_m\}$. That is, Eq. (15). But it is difficult to determine $\beta = (\nu_1, \nu_2, \ldots, \nu_m)$ in Eq. (15). It is also possible to exist a few β's satisfying this formula. For the bipartite graph G_1 illustrated in Figure 1(a), $C(G_1) = 1, C(G_1 - e_1) = C(G_1 - e_2) = C(G_1 - e_3) = C(G_1 - e_4) = 0, C(G_1 - e_5) = 2, C(G_1 - e_6) = C(G_1 - e_7) = 1$. Hence for $\beta = (1,1,1,1,1,1,1), (-1,-1,-1,-1,1,1,1), \ldots,$ Eq.(15) holds. For the bipartite graph G_2 illustrated in Figure 1(b), $C(G_2) = 1, C(G_2 - e_1) = C(G_2 - e_5) = C(G_2 - e_8) = 1, C(G_2 - e_7) = C(G_2 - e_9) = 2, C(G_2 - e_2) = C(G_2 - e_3) = C(G_2 - e_4) = C(G_2 - e_6) = 0$. Hence for $\beta = (-1,1,1,1,-1,1,1,-1,1), (1,1,1,1,-1,1,-1,1,1), \ldots,$ Eq.(15) holds.

***Acknowledgment*:** The author was supported in part by NSFC Grant (12071180). We are thankful to the anonymous referee for his (or her) revised suggestions.

References

[1] O. Bodroža–Pantić, Algebraic structure count of some cyclic hexagonal-square chains on the Möbius strip, *J. Math. Chem.* **41** (2007) 283–294.

[2] O. Bodroža–Pantić, S. J. Cyvin, I. Gutman, A formula for the algebraic structure count of multiple phenylenes, *MATCH Commun. Math. Comput. Chem.* **32** (1995) 47–58.

[3] E. J. Farrell, S. A. Wahid, On the reconstruction of the matching polynomial and the reconstruction conjecture, *Int. J. Math. Math. Sci.* **10** (1987) 155–162.

[4] O. Bodroža–Pantić, I. Gutman, S. J. Cyvin, Algebraic structure count of some non-benzenoid conjugated polymers, *ACH Models Chem.* **133** (1996) 27–41.

[5] O. Bodroža–Pantić, A. Ilić–Kovačević, Algebraic structure count of angular hexagonal-square chains, *Fibonacci Quart.* **45** (2007) 3–9.

[6] E. M. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, Academic Press, New York, 1980.

[7] D. Cvetković, I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. VII. The role of resonance structures, *J. Chem. Phys.* **61** (1974) 2700–2706.

[8] M. J. S. Dewar, H. C. Longuet–Higgins, The correspondence between the resonance and molecular orbital theories, *Proc. Roy. Soc. London A* **214** (1952) 482–493.

[9] A. Graovac, I. Gutman, The determinant of the adjacency matrix of a molecular graph, *MATCH Commun. Math. Comput. Chem.* **6** (1979) 49–73.

[10] A. Graovac, I. Gutman, N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer–Verlag, Berlin, 1977.

[11] A. Graovac, I. Gutman, N. Trinajstić, T. Živković, Graph theory and molecular orbitals. Application of Sachs theorem, *Theor. Chim. Acta* **26** (1972) 67–78.

[12] I. Gutman, Note on algebraic structure count, *Z. Naturforsch.* **39a** (1984) 794–796.

[13] I. Gutman, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbits, X. The number of Kekulé structures and the thermodynamic stability of conjugated systems, *Tetrahedron* **31** (1975) 143–146.

[14] W. C. Herndon, Resonance theory and the enumeration of Kekulé structures, *J. Chem. Ed.* **51** (1974) 10–15.

[15] D. J. Klein, T. G. Schmalz, S. EI–Basil, M. Randić, N. Trinajstić, Kekulé count and algebraic structure count for unbranched alternant cata–fusenes, *J. Mol. Struct. (Theochem)* **179** (1988) 99–107.

[16] S. A. Wahid, *On the matching polynomials of graphs*, M.Sc. Thesis, Univ. West Indies, St. Augustine (Trinidad), 1983.

[17] C. F. Wilcox, A topological definition of resonance energy, *Croat. Chem. Acta* **47** (1975) 87–94.

[18] C. F. Wilcox, Stability of molecules containing $(4n)$-rings, *Tetrahedron Lett.* **9** (1968) 795–800.

[19] C. F. Wilcox, Stability of molecules containing nonalternant rings, *J. Am. Chem. Soc.* **91** (1969) 2732–2736.

[20] C. F. Wilcox, I. Gutman, N. Trinajstić, Graph theory and molecular orbitals, XI. Aromatic substitution, *Tetradedron* **31** (1975) 147–152.

[21] L. Z. Ye, The vertex graphical condensation for algebraic structure count of molecular graphs, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 579–584.

[22] L. Z. Ye, New variants of Gutman's formulas on the algebraic structure count, *MATCH Commun. Math. Comput. Chem.* **89** (2023) 643–652.