MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **85** (2021) 7-11

ISSN 0340 - 6253

A Lower Bound on the Number of Perfect Matchings in Benzenoid Systems

Fuji Zhang[a] , Yuqing Lin[b,c]

[a]*School of Mathematical Sciences, Xiamen University, Xiamen, Fujian 361005, P. R. China*

[b]*School of Electrical Engineering and Computer Science, University of Newcastle, NSW2308, Australia*

[c]*School of Science, Jimei University, Xiamen, Fujian 361005, P. R. China*

(Received July 7, 2020)

Abstract

The number of perfect matchings in a benzenoid system increases when its size grows. This raises a question on the lower bound of the number of perfect matchings in benzenoid systems. In this paper, we show that this lower bound is 9. Furthermore, we construct an infinite family of benzenoid system whose number of perfect matchings reaches the lower bound.

1 Introduction

A *generalized benzenoid* system is a finite connected subgraph of the infinite hexagonal lattice. It may therefore contain cut vertices or non-hexagonal interior faces. A *benzenoid system* H is a generalized benzenoid system without cut vertices or non-hexagonal interior faces. Benzenoid systems are extensively used in the study of benzenoid hydrocarbons, as they model the carbon atoms skeleton of such molecules. A *perfect matching* of H is a covering of all vertices of H by disjoint edges. Perfect matching is also known as *Kekulé structure* in chemistry. These concepts are important in resonance theory in chemistry [6], they are also used in the study of dimmer problem in statistical physics [5].

Supported by NSFC (Grant No.11771181,11971406)

Corresponding author: `yuqing.lin@newcastle.edu.au`

A bond (an edge in graph theoretical terms) of a benzenoid system G is a *fixed single* (respectively, *fixed double*) bond if it belongs to none (respectively, all) of the perfect matchings of H. A bond is fixed if it is either a fixed single bond or a fixed double bond. A benzenoid system with a perfect matching and without fixed bonds is called *normal*. If a benzenoid system G has fixed bonds then the subgraph induced by all non-fixed bonds of G is the union of disjoint connected components. We denote this induced subgraph by $N(G)$, and call it the unfixed subgraph of H. Clearly, none of the edges in the components of $N(G)$ is fixed, i.e., these components are normal, thus we call these components in $N(G)$ *normal components*. Let $\phi(H)$ be the number of perfect matchings in the benzenoid system H.

In general, the number of perfect matchings increases with the number of hexagons. For example, a hexagonal chain with n hexagons have $n+1$ perfect matchings, and we have the following results known since the 1950s:

Theorem 1. *[2] Let H be a fibonaccene chain with h hexagons; let $a_h = \phi(H)$. Then $a_0 = 1$, $a_1 = 2$, and $a_h = a_{h-1} + a_{h-2}$ for $h \geq 2$.*

Theorem 2. *For a parallelogram hexagonal system $P[h,p]$, we have $\phi(P[h,p]) = C(h+p,p)$, where C(x,y) is the binomial coefficients.*

Theorem 13 in [1] states that

Theorem 3. *[1] Let H be a normal benzenoid system with n hexagons, then $\phi(H) \geq n+1$.*

It is clear that there are large benzenoid systems that do not have perfect matchings. For example, start with a benzenoid system with perfect matching, adding a hexagon to the system where the hexagon shares only two adjacent edges with the system. In this case, effectively, there are three new vertices added to the system, thus the resulting benzenoid system has odd number of vertices, thus no perfect matchings. For benzenoid systems with perfect matchings, we do not have an upper bound for the number of perfect matchings. It is natural to think that the lower bound of the number of perfect matching in benzenoid system increases when the number of hexagons is increased. However, to our surprise, there is a fixed constant lower bound. In this paper we prove this result and provide an extremal graph.

2 Main Results

In [3], P. Hansen and M. Zheng have investigated the number of connected components in $N(H)$, and concluded the following:

Theorem 4. *[3] Let H be a benzenoid system. If H has fixed bonds then it has at least two normal components.*

Theorem 5. *[3] If a benzenoid system H with more than one hexagon, has a normal component which is a single hexagon, then H has at least three normal components.*

For the rest of the paper, we are looking at large benzenoid systems. Using the above theorems, we can show that:

Theorem 6. *Let H be a benzenoid system having perfect matchings. If H has more than 9 hexagons, then $\phi(H) \geq 9$*

Proof. Let H be a benzenoid system with more than 9 hexagons. If there are no fixed bound in the system, then, by Theorem 3, H has at least 10 perfect matchings, for example, when H is a chain. Suppose there are fixed bounds in H, then by the Theorem 4, then there are at least two normal components. If none of the components is single hexagon, then each component has at least 3 perfect matchings, overall, has 9 perfect matchings in H. As stated in Theorem 5, it is possible for a benzenoid system to have three components, in which one of them is a single hexagon. If one of the rest two components is not a single hexagons, then the system has at lease $2 \times 2 \times 3 = 12$ perfect matchings. Now assume all three components are single hexagons. There are two cases to consider.

Case 1: If one of the components (which is a single hexagon) is on the boundary of H, then removing the hexagon and incident fixed bound, the left over is a generalized benzenoid system H'. If it has not cut vertex, i.e. no cut edge, then it is clear that H' has not non-hexagonal internal faces, thus H' is a benzenoid system. Furthermore, we know there are fixed bonds in H', otherwise, the hexagon that we have removed have at most 5 hexagons adjacent to it, plus the two normal components which are 2 hexagons, totally we have only 8 hexagons in H, contradicting to the assumption that H has more than 9 hexagons. As we know that $N(H')$ contains a single hexagon, by Theorem 5, we know that H' has at least 3 normal components, contradicting to our assumption. If H' has a cut vertex, i.e. cut edge e, then this edge must be a fixed bond. To see this, considering $H' - e$ which has two connected components, the number of vertices in both components should have the same parity, i.e. both even or both odd. In case that both components have even vertices, then e has to be fixed single bond, otherwise, e has to be fixed double bond. In either case, e is a fixed bond. Then $H' - e$ has a connected component which is a benzenoid system, it has fixed bond and a single hexagon as the unfixed subgraph. Apply Theorem 5, it is clear that there is another normal component in addition to the three hexagons in $N(H)$, a contradiction. So this case is impossible.

Case 2: Suppose none of the hexagons are on the boundary, thus if we remove all three hexagons and connected fixed bonds, clearly, the resulting graph H' is a general benzenoid system. H' has not cut vertex as none of the hexagons are on the boundary. It was shown in [21] that if a graph different from K_2 (i.e., the graph with two vertices and one edge) and with no cut vertices has a perfect matching then it has at least two perfect matchings. Thus, in H', there is an alternating cycle, i.e. not all bonds are fixed bonds, a contradiction to our assumption. So this case is impossible.

Thus we show that for benzenoid system with perfect matchings and has more than 10 hexagons, the lower bound on the number of perfect matching is $3 \times 3 = 9$. ■

Below is a benzenoid system with fixed double bonds identified.

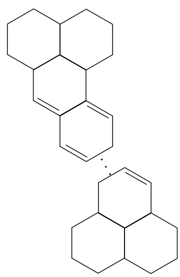

Figure 1. A benzenoid system which has 9 perfect matchings.

It is clear that this benzenoid system has two normal components, each having three perfect matchings. Thus, in total, the system has 9 perfect matchings. Increasing the length of the chain in the middle doesn't increase the number of perfect matching in the system. So the family of the benzenoid system in Fig. 1 achieves the lower bound on the number of perfect matchings.

Corollary 7. *The family of benzenoid systems H in Fig. 1 has $\phi(H) = 9$ which achieves the lower bound on the number of perfect matching.*

References

[1] S. J. Cyvin, I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons*, Springer, Berlin, 1988.

[2] F. J. Rispoli, Counting perfect matchings in hexagonal systems associated with benzenoids, *Math. Magazine* **74** (2001) 194–200.

[3] P. Hansen, M. Zheng, Normal components of benzenoid systems, *Theor. Chim. Acta* **85** (1993) 335–344.

[4] A. Kotzig, On theory of finite graphs with a linear factor I, *Mat. Fyz. Casopis Slovensk. Akad. Vied* **9** (1959) 73–91 (in Slovak).

[5] L. Lováz, M. Plummer, *Matching Theory*, AMS, Providence, 2009.

[6] L. Pauling, *The Nature of the Chemical Bond – An Introduction to Modern Structure Chemistry*, Cornell Univ. Press, Ithaca, 1960.