ELSEVIER

Discrete Applied Mathematics 74 (1997) 191–196

DISCRETE APPLIED MATHEMATICS

Hamilton paths in Z-transformation graphs of perfect matchings of hexagonal systems

Chen Rong-si[a,*], Zhang Fu-ji[b]

[a] College of Finance and Economics, Fuzhou University, Fuzhou, Fujian, 350002, People's Republic of China

[b] Department of Mathematics, Xiamen University, Xiamen, Fujian, 361005, People's Republic of China

Received 26 June 1994; revised 26 March 1996

Abstract

Let H be a hexagonal system. The Z-transformation graph $Z(H)$ is the graph where the vertices are the perfect matchings of H and where two perfect matchings are joined by an edge provided their symmetric difference is a hexagon of H (Z. Fu-ji et al., 1988). In this paper we prove that $Z(H)$ has a Hamilton path if H is a catacondensed hexagonal system.

A hexagonal system [11], also called honeycomb system or hexanimal (see, eg. [10]) is a finite connected plane graph with no cut-vertices, in which every interior region is surrounded by a regular hexagon of side length 1. Hexagonal systems are of chemical significance since a hexagonal system with perfect matchings is the skeleton of a benzenoid hydrocarbon molecule [9]. Recall that a perfect matching of a graph G is a set of disjoint edges of G covering all the vertices of G. In the following discussion we confine our considerations to those hexagonal systems with at least one perfect matching.

Let H be a hexagonal system. The Z-transformation graph $Z(H)$ [3, 4] is the graph where the vertices are the perfect matchings of H and where two perfect matchings M_1 and M_2 are joined by an edge provided their symmetric difference $M_1 \triangle M_2$, i.e. $(M_1 \cup M_2) - (M_1 \cap M_2)$, is a hexagon of H. Z-transformation graphs have some interesting properties. $Z(H)$ is either a path or a bipartite graph with girth 4, and the connectivity of $Z(H)$ is equal to the minimum degree of the vertices of $Z(H)$ [3, 4]. Furthermore, $Z(H)$ has at most two vertices of degree one [3]. The construction feature for the class of hexagonal systems whose Z-transformation graphs have at least one vertex of degree one was reported in [5]. Z-transformation graphs are useful

* Corresponding author.

PII S0166-218X(96)00033-9

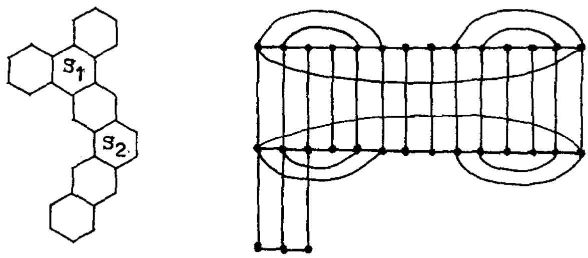


Fig. 1. A catacondensed hexagonal system H with two turning hexagons s_1 and s_2, and the Z-transformation graph $Z(H)$.

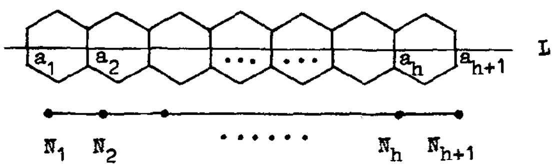


Fig. 2.

in certain enumeration techniques for hexagonal systems [6]. By using the concept of Z-transformation graphs, a class of hexagonal systems with forcing edges is also characterized [7]. In the present paper we prove that for a catacondensed hexagonal system H, $Z(H)$ has a Hamilton path.

Recall that a catacondensed hexagonal system is a hexagonal system whose vertices are all on the perimeter [9]. A hexagon of a catacondensed hexagonal system is said to be a turning hexagon if it has two or three non-parallel edges which are common edges with other hexagons (cf. Fig. 1).

Lemma 1. *Let G be a catacondensed hexagonal system without turning hexagon. Then $Z(G)$ is a path.*

Proof. Since G has no turning hexagon, the centres of the hexagons of G all lie on the line L (see Fig. 2). It is not difficult to check that G has exactly $h + 1$ perfect matchings (cf. [2, p. 38]), each of which has exactly one edge intersected by the line L. Therefore, $Z(G)$ is a path P, the ith vertex of P corresponds to the perfect matching N_i of G containing the edge a_i $(i = 1, 2, \ldots, h + 1)$ (see Fig. 2).

Definition 2 (*J. A. Bondy and U. S. R. Murty* [1]). Let $G_i = (V(G_i), E(G_i))$ be a graph $(i = 1, 2)$. The product $G_1 \times G_2$ is the graph with vertex set $V(G_1 \times G_2) = \{(u, v) \mid u \in V(G_1), v \in V(G_2)\}$, in which (u, v) is adjacent to (u', v') if and only if either $u = u'$ and $vv' \in E(G_2)$ or $v = v'$ and $uu' \in E(G_1)$.

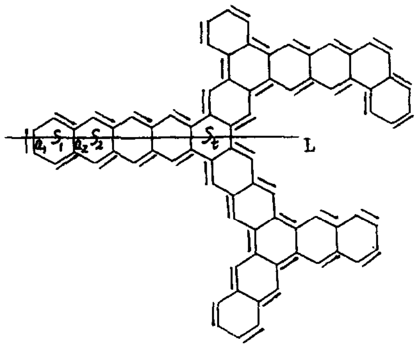


Fig. 3. A catacondensed hexagonal system G and the perfect matching N (its edges are identified by double lines) with all its edges on the perimeter of G.

Lemma 3. *Let $G_i = (V(G_i), E(G_i))$ $(i = 1, 2)$ be a graph with a Hamilton path P_i. Then $G_1 \times G_2$ has a Hamilton path.*

Proof. suppose that $|V(G_1)| = m$, $|V(G_2)| = n$; and $P_1 = u_1u_2 \dots u_m$, $P_2 = v_1v_2 \dots v_n$. Evidently, $(u_1, v_1)(u_2, v_1) \dots (u_m, v_1)(u_m, v_2)$ $(u_{m-1}, v_2) \dots (u_1, v_2)(u_1, v_3) \dots (u_m, v_3) \dots$ is a Hamilton path of $G_1 \times G_2$, in which the last vertex is (u_1, v_n) if n is even or (u_m, v_n) if n is odd. □

Let G be a catacondensed hexagonal system, $s_1, s_2, \dots, s_t$ be hexagons of G, where s_i and s_{i+1} have the edge a_{i+1} in common, and s_t is a turning hexagon as shown in Fig. 3. It is known that G has a perfect matching with all its edges on the perimeter of G since the perimeter of G is a Hamilton cycle of G [8] (cf. Fig. 3). Moreover, each perfect matching of G has exactly one edge intersected by the horizontal line L (see Fig. 3) (cf. [11]). Therefore, we can divide the set of all perfect matchings of G into $t + 1$ disjoint subsets $K_1(G), K_2(G), \dots, K_t(G), K_{t+1}(G)$; where $K_i(G)$ is the set of perfect matchings of G containing the edge a_i $(i = 1, 2, \dots, t + 1)$ (cf. Fig. 4). It is not difficult to see that the perfect matchings of $K_i(G)$ have some other common edges besides the edge a_i $(i = 1, 2, \dots, t + 1)$. We denote the set of the common edges of the perfect matchings of $K_i(G)$ by $M_i(G)$. For $i = 1, 2, \dots, t$, the edges e and f as well as a_{t+1} (see Fig. 4) do not belong to any perfect matching of $K_i(G)$. Let G_1 and G_2 be the components obtained from G by deleting the edges e, f and a_{t+1}, where G_i $(i = 1, 2)$ contains the edge a_1^* (see Fig. 4). Suppose that the numbers of perfect matchings of G_1 and G_2 are p and q, respectively. Then we have $|K_i(G)| = pq$ for $i = 1, 2, \dots, t$. Moreover, each perfect matching of $K_i(G)$ $(i = 1, 2, \dots, t)$ has the form $M_i(G) \cup N_{1j} \cup N_{2r}$, where N_{1j} and N_{2r} are perfect matchings of G_1 and G_2, respectively.

Lemma 4. *Let G be a catacondensed hexagonal system with exactly one turning hexagon. Then $Z(G)$ has a Hamilton path P. Moreover, the first pq vertices of P correspond to the perfect matchings of $K_1(G)$.*

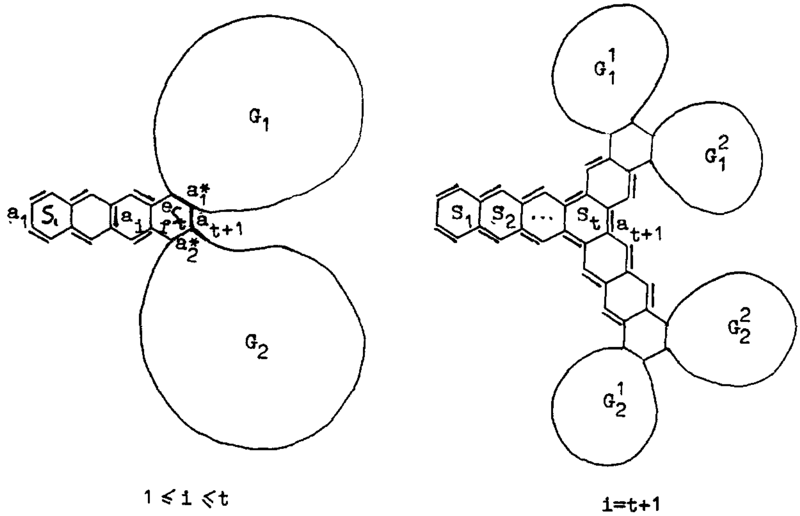


Fig. 4. The common edges of the perfect matchings of $K_i(G)$.

Proof. Since G has exactly one turning hexagon, G_1 and G_2 are both catacondensed hexagonal systems without turning hexagon, or one of them is an edge and the other is a catacondensed hexagonal system without turning hexagon. It suffices to prove the assertion for the former, and the latter can be dealt with fully analogously.

By Lemma 1, $Z(G_1)$ is a Hamilton path $P_1^* = N_{11}N_{12}\ldots N_{1p}$, where N_{11} is the perfect matching of G_1 containing the edge a_1^* (cf. Fig. 4). Similarly, $Z(G_2)$ is a Hamilton path $P_2^* = N_{21}N_{22}\ldots N_{2q}$, where N_{21} is the perfect matching of G_2 containing the edge a_2^*. By Lemma 3, $Z(G_1)\times Z(G_2)$ has a Hamilton path. Since the subgraph $\langle K_i(G)\rangle$ of $Z(G)$ induced by $K_i(G)$ is isomorphic to $Z(G_1)\times Z(G_2)$, $\langle K_i(G)\rangle$ has a Hamilton path P_i *for* $i = 1,2,\ldots,t$. More precisely, the jth vertex of p_i ($i = 1, 2, \ldots, t$) is $M_i(G)\cup N_{1,p+1-r}\cup N_{2,h+1}$, when h is odd; and $M_i(G)\cup N_{1r}\cup N_{2,h+1}$ when h is even; where $j = hp + r$, h and r are positive integers, $0 \leqslant h \leqslant q-1$, $1 \leqslant r \leqslant p$. Now consider the induced subgraph $\langle K_{t+1}(G)\rangle$. Evidently, $M_{t+1}(G)$ is the only member of $K_{t+1}(G)$. It is not difficult to see that $M_{t+1}(G)$ is adjacent to the first vertex of P_t, i.e. $M_t(G)\cup N_{11}\cup N_{21}$, since $M_{t+1}(G)\,\Delta\,(M_t(G)\cup N_{11}\cup N_{21}) = s_t$ (cf. Fig. 4). Note that in $Z(G)$, for each vertex of P_1, say, $M_1(G)\cup N_{1j}\cup N_{2k}$, there is a path $(M_1(G)\cup N_{1j}\cup N_{2k})(M_2(G)\cup N_{1j}\cup N_{2k})(M_3(G)\cup N_{1j}\cup N_{2k})\ldots(M_t(G)\cup N_{1j}\cup N_{2k})$, since $(M_f(G)\cup N_{1j}\cup N_{2k})\,\Delta\,(M_{f+1}(G)\cup N_{1j}\cup N_{2k}) = s_f$ for $f = 1,\ldots,t$. For brevity, we denote the jth vertex in P_i by B_{ij} ($i = 1,2,\ldots,t; j = 1,2,\ldots,pq$). Now we find a Hamilton path in $Z(G)$ as follows: $B_{11}B_{12}\ldots B_{1,pq}\ B_{2,pq}B_{2,pq-1}\ldots B_{21}\ B_{31}\ldots B_{3,pq}\ldots B_{t,pq}B_{t,pq-1}\ldots B_{t1}M_{t+1}(G)$ when t is even; or $B_{1,pq}B_{1,pq-1}\ldots B_{11}B_{21}B_{22}\ldots B_{2,pq}B_{3,pq}\ldots B_{31}\ldots B_{t,pq}B_{t,pq-1}\ldots B_{t1}M_{t+1}(G)$ when t is odd. Evidently, the first pq vertices of the above Hamilton path correspond to the perfect matchings of $K_1(G)$.

We are now in a position to formulate our main theorem.

Theorem 5. *Let G be a catacondensed hexagonal system. Then $Z(G)$ has a Hamilton path with the first pq vertices corresponding to the perfect matchings of $K_1(G)$.*

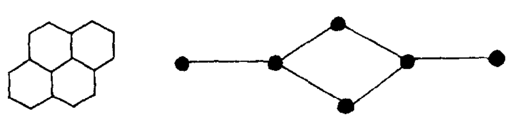
Proof. If G has no turning hexagon, $Z(G)$ itself is a path (Lemma 1). Now suppose that G has at least one turning hexagon. We proceed by induction on the number of turning hexagons.

If G has exactly one turning hexagon, by Lemma 4, the conclusion holds. Assume that G has more than one turning hexagon. As mentioned above, the vertex set of $Z(G)$ is divided into $t+1$ disjoint subsets $K_1(G), K_2(G), \ldots, K_t(G), K_{t+1}(G)$ (cf. Fig. 4). Since G_i ($i = 1,2$) is a catacondensed hexagonal system with fewer turning hexagons than G, by induction hypothesis, $Z(G_i)$ has a Hamilton path P_1^* with the first n_i vertices corresponding to the perfect matchings of $K_1(G_i)$ (i.e. the perfect matchings of G_i containing the edge a_i^*, cf. Fig. 4), where $n_i = |K_1(G_i)|$. Denote $P_i^* = N_{i1}N_{i2} \ldots N_{in_i} \ldots N_{ic_i}$ $(i = 1,2)$. By Lemma 3, $Z(G_1) \times Z(G_2)$ has a Hamilton path $P' = T_1T_2 \ldots T_c$ $(c = c_1c_2)$, where for $j = ac_1 + b$ $(0 < a < c_2 - 1,\ 1 < b < c_1)$, $T_j = (N_{1,c_1+1-b}, N_{2,a+1})$ when a is odd; and $T_j = (N_{1,b}, N_{2,a+1})$ when a is even. Since the subgraph $\langle K_i(G) \rangle$ of $Z(G)$ induced by $K_i(G)$ is isomorphic to $Z(G_1) \times Z(G_2)$, $\langle K_i(G) \rangle$ has a Hamilton path $P_i = D_{i1}D_{i2} \ldots D_{ic}$ for $i = 1,2,\ldots,t$; where $D_{ij} = M_i(G) \cup N_{1,c_1+1-b} \cup N_{2,a+1}$ when a is odd; and $D_{ij} = M_i(G) \cup N_{1,b} \cup N_{2,a+1}$ when a is even; $j = ac_1 + b$, $0 \leqslant a \leqslant c_2 - 1$, $1 \leqslant b \leqslant c_1$. One can check that for each vertex D_{1j} of P_1, there is a path in $Z(G)$: $D_{1j}D_{2j} \ldots D_{tj}$ $(j = 1,2,\ldots,c)$ since $D_{hj} \triangle D_{h+1,j} = M_h(G) \triangle M_{h+1} = s_h$ (cf. Fig. 4), $h = 1,\ldots,t-1$.

Now consider $\langle K_{t+1}(G) \rangle$. Let $N'_{ij} = N_{ij} - M_1(G_i)$, $i = 1,2$; $j = 1,2,\ldots,n_i$; $M_1(G_i)$ is the set of common edges of the perfect matchings of $K_1(G_i)$. Evidently, $\{N'_{ij} \mid j = 1,2,\ldots,n_i\}$ is the set of perfect matchings of $G_i^1 \cup G_i^2$. Hence $Z(G_i^1 \cup G_i^2)$ has a Hamilton path $P'_i = N'_{i1} \cdot N'_{i2} \ldots N'_{in_i}$ $(i = 1,2)$. By Lemma 3, $Z(G_1^1 \cup G_1^2) \times Z(G_2^1 \cup G_2^2)$ has a Hamilton path $\bar{P} = J_1J_2 \ldots J_{n_1n_2}$, where $J_1 = (N'_{11}, N'_{21})$. Since $\langle K_{t+1}(G) \rangle$ is isomorphic to $Z(G_1^1 \cup G_1^2) \times Z(G_2^1 \cup G_2^2)$, $\langle K_{t+1}(G) \rangle$ has a Hamilton path $P_{t+1} = O_1O_2 \ldots O_{n_1n_2}$, where $O_1 = M_{t+1}(G) \cup N'_{11} \cup N'_{21}$. One can check that $O_1 \triangle D_{t1} = (M_{t+1}(G) \cup N'_{11} \cup N'_{21}) \triangle (M_1(G) \cup N_{11} \cup N_{21}) = s_t$. This means that the first vertex of P_{t+1} is adjacent to the first vertex of P_t. Now we find a Hamilton path of $Z(G)$ as follows: $P = D_{11}D_{12} \ldots D_{1c}D_{2c}D_{2,c-1} \ldots D_{21}D_{31} \ldots D_{3c} \ldots D_{tc}D_{t,c-1} \ldots D_{t1}O_1O_2 \ldots O_{n_1n_2}$ when t is even; or $P = D_{1c}D_{1,c-1} \ldots D_{11}D_{21} \ldots D_{2c}D_{3c} \ldots D_{tc}D_{t,c-1} \ldots D_{t1}O_1O_2 \ldots O_{n_1n_2}$ when t is odd.

Remark 6. In the proof of the above theorem, if G_i or G_i^j $(i = 1,2; j = 1,2)$ is exactly an edge, it can be dealt with similarly.

Remark 7. For a hexagonal system which is not catacondensed, its Z-transformation graph need not have a hamilton path. An example is given below.



G Z(G)

Acknowledgements

The authors are indebted to the referee for the valuable comments.

References

[1] J.A. Bondy and U.S.R. Murty, Graph Theory with Applications (North-Holland, Amsterdam, 1981).
[2] S.J. Cyvin and I. Gutman, Kekulé structures in Benzenoid Hydrocarbons (Springer, Berlin, 1988).
[3] Z. Fu-ji, G. Xiaofeng and C. Rong-si, Z-transformation graphs of perfect matchings of hexagonal systems, Discrete Math. 72 (1988) 405–415.
[4] Z. Fu-ji, G. Xiao-feng and C. Rong-si, The connectivity of Z-transformation graphs of perfect matchings of hexagonal systems, Acta Math. Appl. Sinica 4(2) (1988) 131–135.
[5] Z. Fu-ji and G. Xiao-feng, The classification of the hexagonal systems by their Z-transformation, J. Xinjiang University 4(3) (1988) 9–16.
[6] Z. Fu-ji and G. Xiao-feng, The enumeration of several classes of hexagonal systems, to appear.
[7] Z. Fu-ji and L. Xue-liang, Hexagonal systems with forcing edges, Discrete Math., accepted for publication.
[8] I. Gutman, Covering hexagonal systems with hexagons, in: Graph Theory, D. Cvetković, I. Gutman, T. Pisanski and R. Tošić, eds., Proceedings of the Fourth Yugoslav Seminar held at Novi Sad, 1983. (Univerzitet u Novom Sadu, Institut za Mathematiku, Novi Sad, 1984).
[9] I. Gutman and S.J. Cyvin, Introduction to the Theory of Benzenoid Hydrocarbons (Springer, Berlin, 1989).
[10] F. Harary, The cell growth problem and its attempted solutions, in: H. Sachs, H-J. Voss and H. Walther, eds., Beitrage zur Graphentheorie (Int. Koll. Manebach, 9–12, Mai, 1967), (B. G. Teubner Verlagsgesellschaft, Leipzig, 1968) 49–60.
[11] H. Sachs, Perefect matchings in hexagonal systems, J. Combin. 4 (1984) 89–99.