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...
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 $i$th 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 $V(G_1 \times G_2) = \{(u, v) | u \in V(G_1), v \in V(G_2)\}$, 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. 1.* A catacondensed hexagonal system $H$ with two turning hexagons $s_1$ and $s_2$, and the Z-transformation graph $Z(H)$.

*Fig. 2.*
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 $P_1 = u_1 u_2 \ldots u_m, P_2 = v_1 v_2 \ldots v_n$. Evidently, $(u_1, v_1)(u_2, v_1) \ldots (u_m, v_1)(u_m, v_2) (u_{m-1}, v_2) \ldots (u_1, v_2)(u_1, v_3) \ldots (u_m, v_3) \ldots$ 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, $s_1, s_2, \ldots, s_t$ 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 $K_1(G), K_2(G), \ldots, K_t(G), K_{t+1}(G)$; where $K_i(G)$ is the set of perfect matchings of $G$ containing the edge $a_i (i = 1, 2, \ldots, t + 1)$ (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 $a_i (i = 1, 2, \ldots, t + 1)$. We denote the set of the common edges of the perfect matchings of $K_i(G)$ by $M_i(G)$. For $i = 1, 2, \ldots, t$, the edges $e$ and $f$ as well as $a_{i+1}$ (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 $a_{i+1}$, where $G_i (i = 1, 2)$ contains the edge $a_i^* (i = 1, 2, \ldots, t).$ 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 $i = 1, 2, \ldots, t$. Moreover, each perfect matching of $K_i(G) (i = 1, 2, \ldots, t)$ 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 $K_1(G)$. 
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 $\langle K_t(G) \rangle$ of $Z(G)$ induced by $K_t(G)$ is isomorphic to $Z(G_1) \times Z(G_2)$, $\langle K_t(G) \rangle$ has a Hamilton path $P_i$ for $i = 1, 2, \ldots, t$. More precisely, the $j$th vertex of $P_i$ ($i = 1, 2, \ldots, t$) is $M_i(G) \cup N_{1j}N_{2j+1}$, when $h$ is odd; and $M_i(G) \cup N_{1h}N_{2h+1}$ when $h$ is even; where $j = hp + r$, $h$ and $r$ are positive integers, $0 < h < q - 1$, $1 \leq r \leq p$. 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 $P_i$, i.e. $M_i(G) \cup N_{11}N_{21}$, since $M_{t+1}(G) \Delta (M_i(G) \cup N_{11}N_{21}) = s_f$ (cf. Fig. 4). Note that in $Z(G)$, for each vertex of $P_i$, say, $M_i(G) \cup N_{1j}N_{2k}$, there is a path $(M_1(G) \cup N_{1j}N_{2k})(M_2(G) \cup N_{1j}N_{2k})(M_3(G) \cup N_{1j}N_{2k}) \ldots (M_i(G) \cup N_{1j}N_{2k})$, since $(M_f(G) \cup N_{1j}N_{2k}) \Delta (M_{t+1}(G) \cup N_{1j}N_{2k}) = s_f$ for $f = 1, \ldots, t$. For brevity, we denote the $j$th 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: $B_{11}B_{12} \ldots B_{1pq}B_{2pq}B_{2pq-1} \ldots B_{21}B_{3pq} \ldots B_{t, pq}B_{t, pq-1} \ldots B_{11}M_{t+1}(G)$ when $t$ is even; or $B_{11}B_{1pq}B_{1, pq-1} \ldots B_{11}B_{2pq}B_{2pq-1} \ldots B_{21}B_{3pq} \ldots B_{t, pq}B_{t, pq-1} \ldots B_{11}M_{t+1}(G)$ when $t$ is odd. Evidently, the first $pq$ vertices of the above Hamilton path correspond to the perfect matchings of $K_t(G)$.

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 $P_i^*$ with the first $n_i$ vertices corresponding to the perfect matchings of $K_i(G)$ (i.e. the perfect matchings of $G_i$ containing the edge $a^*$, cf. Fig. 4), where $n_i = |K_i(G_i)|$. Denote $P^* = N_1N_2 \ldots N_{n_1}N_{n_2} \ldots N_{n_t}N_{n_{t+1}} (i = 1, 2)$. 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 $j = ac_1 + b$ ($0 < a < c_2 - 1, 1 < b < c_1$), $T_j = (N_1, b, N_2, a + 1)$ when $a$ is odd; and $T_j = (N_1, b, N_2, a + 1)$ when $a$ is even. Since the subgraph $\langle K_t(G) \rangle$ of $Z(G)$ induced by $K_t(G)$ is isomorphic to $Z(G_1) \times Z(G_2)$, $\langle K_t(G) \rangle$ has a Hamilton path $P_t = D_1D_2 \ldots D_{t+1}$ for $i = 1, 2, \ldots, t$; where $D_{ij} = M_i(G) \cup N_1, b \cup N_2, a + 1$ when $a$ is odd; and $D_{ij} = M_i(G) \cup N_1, b \cup N_2, a + 1$ when $a$ is even; $j = ac_1 + b, 0 < a < c_2 - 1, 1 < b < c_1$. One can check that for each vertex $D_{ij}$ of $P_t$, there is a path in $Z(G)$: $D_{ij}D_{i+1} \ldots D_{ij}$ since $D_{ij} \triangle D_{i+1}D_{ij} = M(G) \triangle M_{i+1} = s_i$ (cf. Fig. 4), $h = 1, \ldots, t - 1$.

Now consider $\langle K_{t+1}(G) \rangle$. Let $N''_i = N_i - M_i(G_i), i = 1, 2; j = 1, 2, \ldots, n_i; M_i(G_i)$ is the set of common edges of the perfect matchings of $K_i(G_i)$. Evidently, $\{N''_i | j = 1, 2, \ldots, n_i\}$ is the set of perfect matchings of $G_t \cup G_f$. Hence $Z(G_t \cup G_f)$ has a Hamilton path $P' = N''_1N''_2 \ldots N''_{n_t} (i = 1, 2)$. By Lemma 3, $Z(G_t \cup G_f) \times Z(G_1 \cup G_2)$ has a Hamilton path $P = J_1J_2 \ldots J_{n+1}$, where $J_1 = (N''_1, N''_2)$. Since $\langle K_{t+1}(G) \rangle$ is isomorphic to $Z(G_1 \cup G_f) \times Z(G_1 \cup G_2)$, $\langle K_{t+1}(G) \rangle$ has a Hamilton path $P_{t+1} = O_1O_2 \ldots O_{n+2}$, where $O_1 = M_{t+1}(G) \cup N_{11} \cup N_{21}$. One can check that

Remark 6. In the proof of the above theorem, if $G_i$ or $G_f$ ($i = 1, 2; j = 1, 2$) 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.
Acknowledgements

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

References