Hamilton Cycles in Digraphs of Unitary Matrices

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Abstract

A set $S \subseteq V$ is called an q^+ -set $(q^-$ -set, respectively) if S has at least two vertices and, for every $u \in S$, there exists $v \in S, v \neq u$ such that $N^+(u) \cap N^+(v) \neq \emptyset$ $(N^-(u) \cap N^-(v) \neq \emptyset$, respectively). A digraph D is called *s*-quadrangular if, for every q^+ -set S, we have $| \cup \{N^+(u) \cap N^+(v) : u \neq v, u, v \in S\}| \geq |S|$ and, for every q^- set S, we have $| \cup \{N^-(u) \cap N^-(v) : u, v \in S\}\} \geq |S|$. We conjecture that every strong s-quadrangular digraph has a Hamilton cycle and provide some support for this conjecture.

Keywords: digraph, Hamilton cycle, sufficient conditions, conjecture, quantum mechanics, quantum computing.

1 Introduction

For a digraph D = (V, A) and $x \neq y \in V$, we say that x dominates y, denoted $x \rightarrow y$, if $xy \in A$. All vertices dominated by x are called the *out-neighbors* of x; we denote the set of out-neighbors by $N^+(x)$. All vertices that dominate x are *in-neighbors* of x; the set of in-neighbors is denoted by $N^-(x)$. The number of out-neighbors (in-neighbors) of x is the *out-degree* $d^+(x)$ of x (*in-degree* $d^-(x)$ of x). The maximum semi-degree $\Delta^0(D) = \max\{d^+(x), d^-(x) : x \in V\}$.

A set $S \subseteq V$ is called an q^+ -set $(q^-$ -set, respectively) if S has at least two vertices and, for every $u \in S$, there exists $v \in S, v \neq u$ such that $N^+(u) \cap N^+(v) \neq \emptyset$ $(N^-(u) \cap N^-(v) \neq \emptyset$, respectively). A digraph D is called *s*-quadrangular if, for every q^+ -set S, we have $| \cup \{N^+(u) \cap N^+(v) : u \neq v, u, v \in S\}| \geq |S|$ and, for every q^- -set S, we have $| \cup \{N^-(u) \cap N^-(v) : u, v \in S\}\} \geq |S|$.

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A collection of disjoint cycles that include all vertices of D is called a *cycle factor* of D. We denote a cycle factor as the union of cycles $C_1 \cup \cdots \cup C_t$, where the cycles C_i are disjoint and every vertex of D belongs to a cycle C_j . If t = 1, we say that C_1 is a *Hamilton cycle* of D. A digraph with a Hamilton cycle is called *hamiltonian*. Clearly, the existence of a cycle factor is a necessary condition for a digraph to be hamiltonian.

A digraph D is *strong* if there is a path from x to y for every ordered pair x, y of vertices of D. Clearly, a hamiltonian digraph is strong.

A complex $n \times n$ matrix U is unitary if $U \cdot U^{\dagger} = U^{\dagger} \cdot U = I_n$, where U^{\dagger} denotes the conjugate transpose of U and I_n the $n \times n$ identity matrix. The digraph of an $n \times n$ matrix M (over any field) is a digraph on n vertices with an arc ij if and only if the (i, j)-entry of the M is nonzero. A matrix M (over any field) is *irreducible* if there does not exist a permutation matrix P such that PMP^{-1} equals

$$\left[\begin{array}{cc} A & O \\ B & C \end{array}\right]$$

where O is an all-zero matrix, A and C are square matrices and B is an arbitrary matrix. Notice that the digraph of an irreducible matrix is strong. It was shown in [12] that the digraph of a unitary matrix is s-quadrangular. S-quadrangular tournaments were studied in [10]. We believe that the following claim holds:

Conjecture 1.1 Every strong s-quadrangular digraph has a Hamilton cycle.

It follows that if Conjecture 1.1 is true, then the digraph of an irreducible unitary matrix is hamiltonian. Unitary matrices are important in quantum mechanics and, at present, are central in the theory of quantum computation [11]. In particular, we may associate a strong digraph to a quantum system whose unitary evolution allows transitions only along the arcs of the digraph (that is, respecting the topology of the graph, like in discrete quantum walks [1, 8]). Then, if the conjecture is true, the digraph would be necessarily hamiltonian. Moreover, the conjecture is important in the attempt to understand the combinatorics of unitary and unistochastic matrices, see, e.g., [3, 4, 14]. If the conjecture is true, then the digraph of an irreducible weighing matrix has a Hamilton cycle (see [5], for a reference on weighing matrices). Also, since the Kronecker product of unitary matrices preserves unitarity, if K and H are digraphs of irreducible unitary matrices, then their Kronecker product $K \otimes H$ (see [9], for an interesting collection of notions and results on graph products) has a Hamilton cycle provided $K \otimes H$ is strong.

The hamiltonian cycle problem is one of the central problems in graph theory and its applications [2, 6, 13]. Many sufficient conditions were obtained for hamiltonicity of undirected graphs [6] and only a few such conditions are proved for directed graphs [2] (for conjectures on sufficient conditions for hamiltonicity of digraphs, see [2]). This indicates that the asymmetry of the directed case makes the Hamilton cycle problem significantly harder, in a sense.

The complete biorientation of an undirected graph G is a digraph obtained from G by replacing every edge xy by the pair xy, yx of arcs. A graph is *s*-quadrangular if its complete biorientation is s-quadrangular. Certainly, the following is a weakening of Conjecture 1.1:

Conjecture 1.2 Every connected s-quadrangular graph has a Hamilton cycle.

In this paper, we provide some support to the conjectures. In Section 2, we show that if a strong s-quadrangular digraph D has the maximum semi-degree at most 3, then Dis hamiltonian. In our experience, to improve the result by replacing $\Delta^0(D) \leq 3$ with $\Delta^0(D) \leq 4$ appears to be a very difficult task. In Section 3, we show the improved result only for the case of undirected graphs. Even in this special case the proof is fairly non-trivial.

2 Supporting Conjecture 1.1

The existence of a cycle factor is a natural necessary condition for a digraph to be hamiltonian [7]. The following necessary and sufficient conditions for the existence of a cycle factor is well known, see, e.g., Proposition 3.11.6 in [2].

Lemma 2.1 A digraph H has a cycle factor if and only if, for every $X \subseteq V(H)$, $|\cup_{x \in X} N^+(x)| \ge |X|$ and $|\cup_{x \in X} N^-(x)| \ge |X|$.

Using this lemma, it is not difficult to prove the following theorem:

Theorem 2.2 Every strong s-quadrangular digraph D = (V, A) has a cycle factor.

Proof: Let $X \subseteq V$. If X is a q^+ -set, then

$$|X| \le |\cup (N^+(u) \cap N^+(v) : u \ne v, u, v \in X)| \le |\cup_{x \in X} N^+(x)|.$$

If X is not a q^+ -set, then consider a maximal subset S of X, which is a q^+ -set (possibly $S = \emptyset$). Since D is strong every vertex of X dominates a vertex. Moreover, since every vertex of X - S dominates a vertex that is not dominated by another vertex in X, we have $|\bigcup_{x \in X-S} N^+(x)| \ge |X - S|$. Thus,

$$|\cup_{x \in X} N^+(x)| \ge |X - S| + |\cup_{x \in S} N^+(x)| \ge |X - S| + |S| = |X|.$$

Similarly, we can show that $|\bigcup_{x\in X} N^{-}(x)| \ge |X|$ for each $X \subseteq V$. Thus, by Lemma 2.1, D has a cycle factor.

Now we are ready to prove the main result of this section.

Theorem 2.3 If the out-degree and in-degree of every vertex in a strong s-quadrangular digraph D are at most 3, then D is hamiltonian.

Proof: Suppose that D = (V, A) is a non-hamiltonian strong s-quadrangular digraph and for every vertex $u \in V$, $d^+(u), d^-(u) \leq 3$.

Let $F = C_1 \cup \cdots \cup C_t$ be a cycle factor of D with minimum number $t \ge 2$ of cycles. Assume there is no cycle factor $C'_1 \cup \cdots \cup C'_t$ such that $|V(C'_1)| < |V(C_1)|$. For a vertex u on C_i we denote by u^+ (u^-) the successor (the predecessor) of u on C_i . Also, $x^{++} = (x^+)^+$. Since every vertex belongs to exactly one cycle of F these notations define unique vertices. Let u, v be vertices of C_i and C_j , $i \ne j$, respectively and let $K(u, v) = \{uv^+, vu^+\}$. At least one of the arcs in K(u, v) is not in D as otherwise we may replace the pair C_i, C_j of cycles in F with just one cycle $uv^+v^{++} \dots vu^+u^{++} \dots u$, a contradiction to minimality of t.

Since D is strong, there is a vertex x on C_1 that dominates a vertex y outside C_1 . Without loss of generality, we may assume that y is on C_2 . Clearly, $\{x, y^-\}$ is a q^+ -set. Since $K(x, y^-) \not\subset A$ and $x \rightarrow y$, we have $y^- \not\rightarrow x^+$. This is impossible unless $d^+(x) > 2$. So, $d^+(x) = 3$ and there is a vertex $z \notin \{x^+, y\}$ dominated by both x and y^- . Let z be on C_j .

Suppose that $j \neq 1$. Since $K(x, z^-) \not\subset A$ and $x \to z$, we have $z^- \not\to x^+$. Since $\{x, z^-\}$ is a q^+ -set, we have $z^- \to y$. Suppose that $j \geq 3$. Since $z^- \to y$ and $y^- \to z$, we have $K(y^-, z^-) \subset A$, which is impossible. So, j = 2. Observe that $\{x^+, z\}$ is a q^- -set $(x \to x^+ \text{ and } x \to z)$. But $y^- \not\to x^+$ and $z^- \not\to x^+$. Hence, $|N^-(x^+) \cap N^-(z)| = 1$, which is impossible.

Thus, j = 1. Since $K(y^-, z^-) \not\subset A$ and $y^- \to z$, we have $z^- \not\to y$. Since $\{x, z^-\}$ is a q^+ -set, $z^- \to x^+$. By replacing C_1 and C_2 in F with $x^+ x^{++} \dots z^- x^+$ and $xyy^+ \dots y^- zz^+ \dots x$ we get a cycle factor of D, in which the first cycle is shorter than C_1 . This is impossible by the choice of F.

3 Supporting Conjecture 1.2

Let G = (V, E) be an undirected graph and let $f : V \to \mathcal{N}$ be a function, where \mathcal{N} is the set of positive integers. A subgraph H of G is called an *f*-factor if the degree of a vertex $x \in V$ is equal to f(x). Let e(X, Y) denote the number of edges with one endpoint in Xand one endpoint in Y. We write e(X) = e(X, X) to denote the number of edges in the subgraph $G\langle X \rangle$ of G induced by X. The number of neighbors of a vertex x in G is called the *degree* of x and denoted by $d_G(x)$.

The following assertion is the well-known Tutte's f-factor Theorem (see, e.g., Exercise 3.3.16 in [13]):

Theorem 3.1 A graph G = (V, E) has an f-factor if and only if

$$q(S,T) + \sum_{t \in T} (f(t) - d_{G-S}(t)) \le \sum_{s \in S} f(s)$$

for all choices of disjoint subsets S, T of V, where q(S, T) denotes the number of components Q of $G - (S \cup T)$ such that $e(V(Q), T) + \sum_{v \in V(Q)} f(v)$ is odd.

The following lemma is of interest for arbitrary undirected graphs. A 2-factor of G is an f-factor such that f(x) = 2 for each vertex x in G.

Lemma 3.2 If G = (V, E) is a graph of minimum degree at least 2 and with no 2-factor, then we can partition V(G) into S, T, O and R, such that the following properties hold.

- (i): T is independent.
- (ii): $e(R, O \cup T) = 0$.
- (iii): Every connected component in G(O) has an odd number of edges into T.
- (iv): No $t \in T$ has two edges into the same connected component of G(O).
- (v): For every vertex $o \in O$ we have $e(o,T) \leq 1$.
- (vi): There is no edge of $\in E(G)$, where $t \in T$, $o \in O$, such that e(t,S) = 0 and e(o,O) = 0.
- (vii): $|T| |S| \frac{e(T,O) oc(S,T)}{2} > 0$, where oc(S,T) is the number of connected components in G S T, which have an odd number of edges into T. (Note that oc(S,T) is also the number of connected components of $G\langle O \rangle$, by (ii) and (iii).)

Proof: By Tutte's f-factor Theorem, there exists disjoint subsets S and T of V, such that the following holds.

$$oc(S,T) + 2|T| - \sum_{v \in T} d_{G-S}(v) > 2|S|$$

Define

$$w(S,T) = |T| - |S| - e(T) - \frac{e(T, V - S - T) - oc(S,T)}{2}$$

We now choose disjoint subsets S and T of V, such that the following holds in the order it is stated.

• maximize w(S,T)

- minimize |T|
- maximize |S|
- minimize oc(S,T)

Furthermore, let O contain all vertices in V - S - T belonging to connected components of $G\langle V - S - T \rangle$, each of which has an odd number of edges into T. Let R = V - S - T - O. We will prove that S, T, O and R satisfy (i)-(vii).

Clearly, w(S,T) > 0. Let $t \in T$ be arbitrary and assume that t has edges into i connected components in $G\langle O \rangle$. Let S' = S and let $T' = T - \{t\}$. Furthermore let j = 1 if the connected component in $G\langle V - S' - T' \rangle$ containing t has an odd number of edges into T', and j = 0, otherwise. Observe that |T'| = |T| - 1, e(T') = e(T) - e(t,T), e(T', V - S' - T') = e(T, V - S - T) - e(t, V - S - T) + e(t,T) and oc(S',T') = oc(S,T) - i + j. Since |T'| < |T|, we must have w' = w(S',T') - w(S,T) < 0. Therefore, we have

$$w' = -1 + e(t,T) + \frac{e(t,V-S-T) - e(t,T) - i + j}{2} < 0.$$
$$e(t,T) + e(t,V-S-T) - i + j \le 1$$
(1)

Thus,

Observe that, by the definition of i, $e(t, V-S-T) \ge i$. Now, by (1), $i \le e(t, V-S-T) \le i - j - e(t, T) + 1$. Thus, $j + e(t, T) \le 1$ and, if e(t, T) > 0, then e(t, T) = 1, j = 0 and e(t, V-S-T) = i. However, e(t, T) = 1, e(t, V-S-T) = i and a simple parity argument imply j = 1, a contradiction.

So e(t,T) = 0. In this case, e(t, V - S - T) - i = 0 or 1. If e(t, V - S - T) - i = 1, then, by a simple parity argument, we get j = 1, which is a contradiction against (1). Therefore, we must have e(t, V - S - T) = i.

It follows from e(t,T) = 0, e(t,V-S-T) = i, w(S,T) > 0 and the definition of O that (i), (ii), (iv) and (vii) hold. We will now prove that (v) and (vi) also hold. Suppose that there is a vertex $o \in O$ with e(o,T) > 1. Let $S' = S \cup \{o\}$ and T' = T, and observe that

$$w(S',T') - w(S,T) = -1 + (e(o,T) - (oc(S,T) - oc(S',T')))/2 < 0$$
⁽²⁾

If $e(o,T) \geq 3$ then, by (2), oc(S,T) > oc(S',T') + 1. However, by taking *o* from *O*, we may decrease oc(S,T) by at most 1, a contradiction. So, e(o,T) = 2 and, by (2), oc(S,T) > oc(S',T'). However, since e(o,T) is even, taking *o* from *O* will not decrease o(S,T), a contradiction. Therefore (v) holds.

Suppose that there is an edge $ot \in E(G)$, where $t \in T$, $o \in O$, such that e(t, S) = 0 and e(o, O) = 0. Let S' = S and $T' = T \cup \{o\} - \{t\}$. By (iii) and (iv), the connected component in $G\langle V - S' - T' \rangle$, which contains t, has an odd number of arcs into T'. This implies that

oc(S',T') - oc(S,T) = -e(t,O) + 1. Also, e(T,V-S-T) = e(T',V-S'-T') + e(t,O) - 1. By (v) we have e(T') = 0. The above equalities imply that w(S',T') = w(S,T). Since the degree of t is at least 2 and e(t,S) = 0, we conclude that $e(t,O) \ge 2$. Thus, oc(S',T') < oc(S,T), which is a contradiction against the minimality of oc(S,T). This completes that proof of (vi) and that of the lemma.

For a vertex x in a graph G, N(x) denotes the set of neighbors of x; for a subset of X of V(G), $N(X) = \bigcup_{x \in X} N(x)$. A 2-factor contains no cycle of length 2. Thus, the following theorem cannot be deduced from Theorem 2.2. For a vertex x in a graph G, N(x) is the set of neighbors of x.

Theorem 3.3 Every connected s-quadrangular graph with at least three vertices contains a 2-factor.

Proof: Suppose G is a connected s-quadrangular graph with at least three vertices and with no 2-factor. Suppose G has a vertex x of degree 1 such that xy is the only edge entering x. Consider $z \neq x$ adjacent with y. Observe that vertices x, z have a common neighbor, but only one common neighbor. Thus, G is not s-quadrangular. Thus, we may assume that the minimum degree of a vertex in G is at least two and we cause Lemma 3.2.

Let S, T, O and R be defined as in Lemma 3.2. First suppose that there exists a vertex $t \in T$ with e(t, S) = 0. Let $y \in N(t)$ be arbitrary, and observe that $y \in O$, by (i) and (ii). Furthermore observe that $e(y, O) \ge 1$ by (vi), and let $z \in N(y) \cap O$ be arbitrary. Since $y \in N(t) \cap N(z)$, there must exist a vertex $u \in N(t) \cap N(z) - \{y\}$, by the definition of an s-quadrangular graph. However, $u \notin O$ by (iv), $u \notin R$ by (ii), $u \notin T$ by (i), and $u \notin S$ as e(t, S) = 0. This contradiction implies that e(t, S) > 0 for all $t \in T$.

Let $S_1 = \{s \in S : e(s,T) \leq 1\}$ and let $W = T \cap N(S - S_1)$. Observe that for every $w \in W$ there exists a vertex $s \in S - S_1$, such that $w \in N(s)$. Furthermore, there exists a vertex $w' \in T \cap N(s) - \{w\}$, by the definition of S_1 . Note that $w' \in W$, which proves that for every $w \in W$, there is another vertex, $w' \in W$, such that $N(w) \cap N(w') \neq \emptyset$. Let $Z = \bigcup(N(u) \cap N(v) : u \neq v \in W)$. By (i), (ii) and (v), $Z \subseteq S - S_1$. By (ii) and (iii), $oc(S,T) \leq e(T,O)$ and, thus, by (vii), |S| < |T|. Observe that $|N(S_1) \cap T| \leq |S_1|$. The last two inequalities and the fact that e(t,S) > 0 for all $t \in T$ imply $|Z| \leq |S - S_1| < |T - N(S_1)| \leq |W|$. This is a contradiction to the definition of an s-quadrangular graph. \Box

The next theorem is the main result of this section.

Theorem 3.4 If the degree of every vertex in a connected s-quadrangular graph G is at most 4, then G is hamiltonian.

Proof: Suppose that G = (V, E) is not hamiltonian. Let $C_1 \cup C_2 \cup \cdots \cup C_m$ be a 2-factor with the minimum number $m \ge 2$ of cycles. Notice that each cycle C_i is of length at least three.

For a vertex v on C_i , v^+ is the set of the two neighbors of v on C_i . We will denote the neighbors by v_1 and v_2 . The following simple observation is of importance in the rest of the proof:

If u, v are vertices of $C_i, C_j, i \neq j$, respectively, and $uv \in E$, then $e(u^+, v^+) = 0$.

Indeed, if $e(u^+, v^+) > 0$, then by deleting one edge from each of C_i, C_j and adding an edge between u^+ and v^+ and the edge uv, we may replace C_i, C_j by just one cycle, which contradicts minimality of m.

We prove that every vertex u which has a neighbor outside its cycle C_i has degree 4. Suppose d(u) = 3. Let $uv \in E$ such that $v \in C_j$, $j \neq i$. Since u, v_1 must have a common neighbor $z \neq v$, we conclude that $e(u^+, v^+) > 0$, which is impossible.

Since G is connected, there is a vertex $u \in C_1$ that has a neighbor outside C_1 . We know that d(u) = 4. Apart from the two vertices in u^+ , the vertex u is adjacent to two other vertices x, y. Assume that x, y belong to C_i, C_j , respectively. Moreover, without loss of generality, assume that $i \neq 1$. Since x_k (k = 1, 2) and u have a common neighbor different from x, u_1 and u_2 , we conclude that y is adjacent to both x_1 and x_2 . Since d(y) < 5, we have $|\{u, x_1, x_2, y_1, y_2\}| < 5$. Since u, x_1, x_2 are distinct vertices, without loss of generality, we may assume that y_2 is equal to either x_1 or u. If $y_2 = u$, then $y \in u^+$ and x_1 is adjacent to a vertex in u^+ , which is impossible.

Thus, $y_2 = x_1$. This means that the vertices $y_1, y, x_1 = y_2, x, x_2$ are consecutive vertices of C_i . Recall that $x_2y \in E$. Suppose that C_i has at least five vertices. Then $y_1, y_2 = x_1, x_2$ and u are all distinct neighbors of y. Since u_1 and y have a common neighbor different from u, the vertex u_1 is adjacent to either y_1 or y_2 or x_2 , each possibility implying that $e(u^+, x^+) + e(u^+, y^+) > 0$, which is impossible.

Thus, C_i has at most four vertices. Suppose C_i has three vertices: x, y, x_1 . Since u and y must have a common neighbor different from $x, y \in x^+$ is adjacent to a vertex in u^+ , which is impossible. Thus, C_i has exactly four vertices: $y, x_1 = y_2, x$ and $x_2 = y_1$. The properties of u and C_i that we have established above can be formulated as the following general result:

Claim A: If a vertex w belonging to a cycle C_p is adjacent to a vertex outside C_p , then w is adjacent to a pair w' and w'' of vertices belonging to a cycle C_q of length four, $q \neq p$, such that w' and w'' are not adjacent on C_q .

By Claim A, x and y are adjacent not only to u, but also to another vertex $v \notin \{u, u_1, u_2\}$ of C_1 , and C_1 is of length four.

For the vertex set $S = \{u, x_1, x_2\}$ there must be a set T with at least three vertices such

that each $t \in T$ is a common neighbor of a pair of vertices in S. This implies that there must be a vertex $z \notin \{x, y, u_1, u_2, u, v\}$ adjacent to both x_1 and x_2 . Thus, z is on C_k with $k \notin \{1, i\}$. By Claim A, x_1 and x_2 are also adjacent to a vertex s on C_k different from z_1 and z_2 . Continue our argument with z_1 and z_2 and similar pairs of vertices, we will encounter cycles Z_1, Z_2, Z_3, \ldots $(Z_j = z_j^1 z_j^2 z_j^3 z_j^4 z_j^1)$ such that $\{z_j^2 z_{j+1}^1, z_j^4 z_{j+1}^1, z_j^2 z_{j+1}^3, z_j^4 z_{j+1}^3\} \subset E$ for $j = 1, 2, 3, \ldots$. Here $Z_1 = C_1, Z_2 = C_i, Z_3 = C_k$.

Since the number of vertices in G is finite, after a while we will encounter a cycle Z_r that we have encountered earlier. We have $Z_r = Z_1$ since for each m > 1 after we encountered Z_{m+1} we have established all neighbors of the vertices in Z_m . This implies that $z_1^1 z_1^2 z_1^3 z_1^4 z_2^1 z_2^2 z_2^3 z_2^4 \dots z_{r-1}^1 z_{r-1}^2 z_{r-1}^3 z_{r-1}^4 z_1^1$ is a cycle of G consisting of the vertices of the cycles Z_1, Z_2, \dots, Z_{r-1} . This contradicts minimality of m.

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