Upper Hamiltonian Numbers and Hamiltonian Spectra of Graphs

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Abstract

If π is a cyclic order of the vertices of a graph G, the number $h(\pi)$ is defined to be the sum of the distances between consecutive vertices of G in π. For a graph G, the hamiltonian spectrum $\mathcal{H}(G)$ is the set of all numbers $h(\pi)$. The hamiltonian number $h(G)$ of G is the minimum number contained in $\mathcal{H}(G)$ and the upper hamiltonian number $h^+(G)$ is the maximum number contained in $\mathcal{H}(G)$. We determine hamiltonian spectra of cycles. We also show that the upper hamiltonian number of a graph G of order n and diameter d is at least $n + \lceil d^2/2 \rceil - 1$. The bound is tight for all pairs n and d.

1 Introduction

A *Hamilton cycle* is a cycle of a graph that contains all the vertices. A graph is called *hamiltonian* if it contains a Hamilton cycle. Hamilton cycles as well

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as necessary and sufficient conditions for their existence form an important part of graph theory (see [4, 5, 8, 12]). A *Hamilton walk* is a closed walk that contains all the vertices of G. Not all graphs contain a Hamilton cycle, however, every connected graph has a Hamilton walk. It is clear that the shortest Hamilton walk has length at least $|V(G)|$ and at most $2|V(G)|-2$, and G has a Hamilton walk of length $|V(G)|$ if and only if G is Hamiltonian. The *hamiltonian number* of G, defined as the length of the shortest Hamilton walk of G, measures how close (far) a graph is to having a Hamilton cycle. The notion of hamiltonian numbers was introduced [9, 10], and has been studied in [1, 2, 3, 11].

The hamiltonian numbers can also be defined using cyclic orders. A *cyclic order* of the vertices of a graph G is a function $\pi : \{1, \ldots, |V(G)|\} \to V(G)$. If $\pi^{-1}(v) = \pi^{-1}(w) + 1$ (the equality is modulo $|V(G)|$), then v is the *successor* of w and w is the *predecessor* of v. Two cyclic orders are the same if they differ only by a rotation and/or a reflection, For a cyclic order π, one may define a corresponding Hamilton walk C_π in G as the union of shortest paths between the vertices consecutive in π. Note that there might be more Hamilton walks C_π corresponding to π, but all of them have the same length. This length is denoted $h(\pi)$, i.e., $h(\pi) = \sum_{i=1}^{n} d_G(\pi(i), \pi(i+1))$. The hamiltonian number of a graph G is then equal to the minimum $h(\pi)$ taken over all the cyclic orders on the vertices of G

The problem of determining numbers $h(\pi)$ for all cyclic orders π of the vertices of a graph G has also been studied. The maximum $h(\pi)$ is called the *upper hamiltonian number* of G and the set $\mathcal{H}(G)$ of all the numbers $h(\pi)$ is called the *hamiltonian spectrum* of G. It was proved in [6, 7] that the upper hamiltonian number of a path P_n is $\lfloor n^2/2 \rfloor$ and that of an odd cycle C_{2k+1} is $2k^2 + k$. In the case of even cycles, Chartrand et al. [7, Conjecture 4.3] conjectured that $h^+(C_{2k}) = 2k^2 - 2k + 2$. In this paper, we prove this conjecture. Moreover, we determine the hamiltonian spectra of cycles of all lengths.

Lower bounds on the upper hamiltonian numbers in terms of the order and the diameter of a graph was discussed in [6]. It was proved there that if G is a graph of order n and diameter d, then the following holds:

$$h^+(G) \geq \begin{cases} n + d - 1 & \text{if } d = 1 \text{ or } d = 2, \\ n + d + 1 & \text{if } d = 3, \\ n + \binom{d}{2} + 1 & \text{otherwise.} \end{cases}$$

Chartrand et. al. [6] expected the bound not to be tight for $d \geq 4$. Indeed, the bound can be improved. In Section 5, we show that $h^+(G) \geq n + \lceil d^2/2 \rceil - 1$. Our bound is tight for all pairs of n and d.

Let us remark that determining the upper hamiltonian number of a graph is an NP-hard problem: for a graph G of order n, consider the graph G' obtained from the complement of G by adding a new vertex v and joining v to all the vertices of G. It is easy to see that $h^+(G') = 2(n-1)+2$ if G has a Hamilton path, and $h^+(G') < 2(n-1)+2$, otherwise.

2 Upper Hamiltonian Numbers of Even Cycles

In this section, we study the upper hamiltonian numbers of even cycles and settle Conjecture 4.3 posed in [7].

Theorem 1. *The upper hamiltonian number of the cycle C_{2k}, $k \geq 2$, is $2k^2 - 2k + 2$.*

Proof. Chartrand et. al. [7] showed that $h^+(C_{2k}) \geq 2k^2 - 2k + 2$. We focus on proving that the bound is tight. The proof proceeds by induction on k. If $k = 2$, it can be easily verified that $h^+(C_4) = 6$. Let us assume that $k > 2$ in the rest. We show that $h(\pi) \leq 2k^2 - 2k + 2$ for each cyclic order π of the vertices of C_{2k}. The statement of the theorem then follows.

Let $v_1, \ldots, v_{2k}$ be the vertices of C_{2k} in the order along the cycle. If the following holds

$$d(\pi(i), \pi(i+1)) + d(\pi(i+1), \pi(i+2)) \leq 2k - 2 \tag{1}$$

for every $i = 1, \ldots, 2k$ (indices are modulo $2k$ where appropriate), then summing up (1) over all $i = 1, \ldots, 2k$ yields:

$$2h(\pi) = \sum_{i=1}^{2k} \left(d(\pi(i), \pi(i+1)) + d(\pi(i+1), \pi(i+2))\right) \leq 2k(2k-2).$$

The bound on $h(\pi)$ follows.

Thus we assume that the inequality (1) does not hold for some i. By symmetry, we can assume that it does not hold for $i = 1$ and that $\pi(1) = v_1$, $\pi(2) = v_{k+1}$ and $\pi(3) = v_2$. In particular, $d(\pi(1), \pi(2)) = k$ and $d(\pi(2), \pi(3)) = k - 1$. Let C' be the cycle obtained from C_{2k} by deleting v_1

and v_{k+1} and by adding edges $v_{2k}v_2$ and v_kv_{k+2}. Clearly, C' is a cycle of length $2(k-1)$. Consider the cyclic order $\pi'(i) = \pi(i+2)$, $i = 1, \dots, 2k-2$, of the vertices of C'. By the induction hypothesis, $h(\pi') \leq 2(k-1)^2 - 2(k-1) + 2 = 2k^2 - 6k + 6$.

In the rest, the vertices $v_2, v_3, \dots, v_k$ are called *red* and the vertices $v_{k+2}, \dots, v_{2k}$ *blue*. The vertices v_1 and v_{k+1} do not have any color. It is easy to see that the distance between vertices of different colors in C_{2k} is the distance between them in C' increased by one. The distances in C_{2k} and C' between the pairs of vertices of the same color are the same. Hence, the number $h(\pi)$ is equal to $h(\pi')$ increased by $2k-1$ (because of the missing terms $d(\pi(1), \pi(2))$ and $d(\pi(2), \pi(3))$ in the sum), increased by the number of red-blue pairs of consecutive vertices in the sequence $\pi(3), \dots, \pi(2k)$ and increased by one if $\pi(2k)$ is red. The last adjustment corresponds to the difference of $d(\pi(2k), \pi(1))$ in C_{2k} and $d(\pi'(2k-2), \pi'(1))$ in C'. There are at most $2k-3$ red-blue pairs of consecutive vertices in $\pi(3), \dots, \pi(2k)$ and if there are $2k-3$ such pairs, then since $\pi(3) = v_2$ is red, $\pi(2k)$ must be blue. Therefore,

$$h(\pi) \leq h(\pi') + 2k - 1 + 2k - 3 \leq 2k^2 - 6k + 6 + 4k - 4 = 2k^2 - 2k + 2.$$

□

We combine Theorem 1 with the results from [7] on the upper hamiltonian numbers of odd cycles to obtain a complete characterization of the upper hamiltonian numbers of cycles:

Corollary 2. *The following equality for the upper hamiltonian number of cycles C_n, $n \geq 3$, holds:*

$$h^+(C_n) = \begin{cases} n^2/2 - n + 2 & \text{if } n \text{ is even,} \\ n^2/2 - n/2 & \text{otherwise.} \end{cases}$$

3 Hamiltonian Spectra of Even Cycles

In this section, we determine the hamiltonian spectra of even cycles. For convenience, in this and the next sections, the vertices of the cycle C_n are always denoted by $v_1, v_2, \cdots, v_n$. We introduce several definitions related to cyclic orders. If π is a cyclic order of the vertices of C_n, then $\pi(i) \pm 1$ denotes the vertex v_j such that $v_{j\mp 1} = \pi(i)$. The (a,b)-*reversion* of π, $a < b$, is the following cyclic order $\pi[a,b]$:

$$\pi[a,b](i) = \begin{cases} \pi(a+b-i) & \text{if } a \le i \le b, \\ \pi(i) & \text{otherwise.} \end{cases}$$

If $a > b$, then the (a,b)-*reversion* of π is the following cyclic order $\pi[a,b]$ (numbers taken modulo the length n of the cycle C_n where appropriate):

$$\pi[a,b](i) = \begin{cases} \pi(i) & \text{if } b < i < a, \\ \pi(b+a-i) & \text{otherwise.} \end{cases}$$

Informally, the reversion $\pi[a,b]$ is obtained by reversing the subsequence between the a-th and the b-th element in the cyclic order. An (a,b)-reversion is said to be *simple* if $\pi(a)$ and $\pi(b)$ are joined by an edge in C_n. We state as a proposition the fact that every two cyclic orders can be obtained from each other by a sequence of simple reversions:

Proposition 3. *Let π and π' be two cyclic orders. There exists a series of simple reversions on π such that the final cyclic order is the same as π'.*

Proposition 3 can be verified using its analogue on transpositions of permutations that is better known: for any two permutations σ and σ', there exists a series of transpositions of consecutive elements that changes σ to σ'. In order to see this, note that $\pi[a,b][b,a]$ differs from π by the transposition of its a-th and the b-th elements and reversing its order.

Lemma 4. *For any cyclic order π of the vertices of a cycle C and for any $1 \le a < b \le n$, if $\pi(a)$ and $\pi(b)$ are neighbors, then $|h(\pi) - h(\pi[a,b])| \le 2$.*

Proof. By symmetry, we can assume $\pi(b) = \pi(a) + 1$. Then

$$\begin{aligned} h(\pi[a,b]) = h(\pi) \quad &- \quad d(\pi(a-1),\pi(a)) - d(\pi(b),\pi(b+1)) \\ &+ \quad d(\pi(a-1),\pi(b)) + d(\pi(a),\pi(b+1)) \end{aligned} \tag{2}$$

Since $\pi(b) = \pi(a)+1$, we have $|d(\pi(a-1),\pi(b)) - d(\pi(a-1),\pi(a))| \le 1$ and $|d(\pi(a),\pi(b+1)) - d(\pi(b),\pi(b+1))| \le 1$. Therefore, $|h(\pi) - h(\pi[a,b])| \le 2$. □

Theorem 5. *If $n \ge 4$ is an even integer, then*

$$\mathcal{H}(C_n) = \{n, n+2, \ldots, n^2/2 - n, n^2/2 - n + 2\}.$$

Proof. Since n is even, each closed walk of C_n has an even length. In particular, $\mathcal{H}(C_n)$ contains no odd numbers. Hence, $h(\pi)$ is even for any π. By Lemma 4, $|h(\pi) - h(\pi[a,b])| = 0$ or 2 for any simple reversion $\pi[a,b]$ of π.

Since $h(C_n) = n$ and $h^+(C_n) = n^2/2 - n + 2$, there exists cyclic orders π and π' of the vertices of C_n such that $h(\pi) = n$ and $h^+(\pi) = n^2/2 - n + 2$. By Proposition 3, π can be changed to π' through a series of simple reversions. At each step, the value $h(\pi)$ is increased or decreased by at most two. Since $\mathcal{H}(C_n)$ contains no odd numbers, it follows that $\mathcal{H}(C_n)$ contains all the even numbers between n and $n^2/2 - n + 2$. □

4 Hamiltonian Spectra of Odd Cycles

In the case of odd cycles, the value $h(\pi) - h(\pi[a,b])$ in Lemma 4 can be -1 or $+1$. Hence, a more careful analysis is needed to determine the hamiltonian spectra of odd cycles. We first establish two auxiliary lemmas.

Lemma 6. *Let C_n be a cycle of odd length n and π a cyclic order of its vertices. If $h(\pi) \leq 2n - 3$, then $h(\pi)$ is odd.*

Proof. Since the length of the cycle is odd, there is a unique shortest path between any two of its vertices. Let P_i, $i = 1, \ldots, n$, be the shortest path between the vertices $\pi(i)$ and $\pi(i+1)$. For an edge e of C_n, let $k(e)$ be the number of the paths P_i that contain the edge e.

Let us consider two distinct edges e and f of C_n. Since the edges e and f form an edge-cut of the cycle C_n and the union of the paths $P_1, \ldots, P_n$ form a closed walk in C_n covering all the vertices, the sum of $k(e)$ and $k(f)$ is an even integer that is at least 2. Therefore, either all the numbers $k(e)$ are even or all of them are odd. In the former case, at most one of the numbers $k(e)$ is equal to zero and the remaining ones are at least two. However, it must then hold that $h(\pi) \geq 2n - 2$. Hence, if $h(\pi) \leq 2n - 3$, all the numbers $k(e)$ must be odd. Consequently, $h(\pi)$ is the sum of an odd number of odd numbers. □

Lemma 7. *If C_n is a cycle of odd length n, then $n^2/2 - n/2 - 1 \notin \mathcal{H}(C_n)$.*

Proof. Let $n = 2k+1$. Assume to the contrary that $h(\pi) = n^2/2 - n/2 - 1 = k(2k+1) - 1$ for a cyclic order π of the vertices of C_{2k+1}. Since the diameter of C_{2k+1} is k, the distance between all the pairs of the consecutive vertices in π except for one is k. By symmetry, we can assume that $d(\pi(1), \pi(2)) =$

$\cdots = d(\pi(2k), \pi(2k+1)) = k$. In addition, we can also assume that $\pi(1) = v_1$ and $\pi(2) = v_{k+2}$. This implies that $\pi(3) = v_2$, $\pi(4) = v_{k+3}$, $\pi(5) = v_3$, etc. In particular, $\pi(2k+1) = v_{k+1}$ and thus $d(\pi(2k+1), \pi(1)) = k$. Consequently, all the distances $d(\pi(i), \pi(i+1))$ are equal to k and $h(\pi) = k(2k+1)$. □

Next, we show that all the numbers between $2n-2$ and $n^2/2-n/2-2$ are contained in the hamiltonian spectrum of the odd cycle C_n. The argument is a little bit more complicated. First we introduce some definitions. Suppose π is a cyclic order of the vertices of C_n. If the shortest path between $\pi(i)$ and $\pi(i+1)$ contains the vertex $\pi(i)+1$, then we call the pair $(\pi(i), \pi(i+1))$ a *forward pair* (with respect to π). Otherwise, the shortest path between $\pi(i)$ and $\pi(i+1)$ contains the vertex $\pi(i)-1$ and the pair $(\pi(i), \pi(i+1))$ is called a *backward pair*. We define the *trace* $t(\pi)$ of π to be the vector $(t_1, \ldots, t_n)$ where t_k, $k = 1, \ldots, n$, is the number of indices $i = 1, \ldots, n$ such that $d(\pi(i), \pi(i+1)) = k$. Note that $h(\pi) = \sum_{k=1}^{n} k \cdot t_k$. The maximum k such that $t_k \neq 0$ is denoted by $t_{\max}(\pi)$ and the pairs $(\pi(i), \pi(i+1))$ with $d(\pi(i), \pi(i+1)) = t_{\max}(\pi)$ are called *long pairs*. The traces of orders can be lexicographically ordered: a trace t is smaller than a trace t' if $t_k < t'_k$ for the largest k such that $t_k \neq t'_k$.

Lemma 8. *Let π be a cyclic order of the vertices of a cycle C_n and let a and b be two indices such that $\pi(a) = \pi(b)-1$. The following statements are true:*

- *If the pairs $(\pi(a), \pi(a+1))$ and $(\pi(b-1), \pi(b))$ of the vertices of C_n are forward and $d(\pi(a), \pi(a+1)) \geq 2$ or $d(\pi(b-1), \pi(b)) \geq 2$, then $h(\pi) - 2 \in \mathcal{H}(C_n)$.*
- *If the pairs $(\pi(a-1), \pi(a))$ and $(\pi(b), \pi(b+1))$ of the vertices of C_n are backward and $d(\pi(a-1), \pi(a)) \geq 2$ or $d(\pi(b), \pi(b+1)) \geq 2$, then $h(\pi) - 2 \in \mathcal{H}(C_n)$.*

Proof. By symmetry, it is enough to prove the first claim of the lemma with $d(\pi(a), \pi(a+1)) \geq 2$. Consider the cyclic order $\pi' = \pi[b, a]$. Since there are only two different pairs of consecutive vertices in the cyclic orders determined by π and π', the following holds:

$$\begin{aligned} h(\pi') = h(\pi) \quad &- \quad d(\pi(a), \pi(a+1)) - d(\pi(b-1), \pi(b)) \\ &+ \quad d(\pi'(a), \pi'(a+1)) + d(\pi'(b-1), \pi'(b)). \end{aligned}$$

However, since both the pairs $(\pi(a), \pi(a+1))$ and $(\pi(b-1), \pi(b))$ are forward, we also have that:

$$\begin{array}{rcccl} d(\pi'(a), \pi'(a+1)) & = & d(\pi(b), \pi(a+1)) & = & d(\pi(a), \pi(a+1)) - 1 \text{ and} \\ d(\pi'(b-1), \pi'(b)) & = & d(\pi(b-1), \pi(a)) & = & d(\pi(b-1), \pi(b)) - 1 \ . \end{array}$$

Therefore, $h(\pi') = h(\pi) - 2$ and $h(\pi) - 2 \in \mathcal{H}(C_n)$. □

Lemma 9. *Let π be a cyclic order of the vertices of C_n whose trace $t(\pi)$ is lexicographically minimal among all the cyclic orders π' with $h(\pi') = h(\pi)$. Assume that the pair $(\pi(a), \pi(a+1))$ is forward and $d(\pi(a), \pi(a+1)) \geq 2$. Let b and b' be two indices such that $\pi(b) = \pi(a)+1$ and $\pi(b') = \pi(a+1)-1$. If $h(\pi) - 2 \notin \mathcal{H}(C_n)$, then the following holds:*

$$\begin{array}{rcl} d(\pi(b-1), \pi(b)) & \geq & d(\pi(a), \pi(a+1)) - 1 \text{ and} \\ d(\pi(b'), \pi(b'+1)) & \geq & d(\pi(a), \pi(a+1)) - 1 \ . \end{array}$$

An analogous statement holds if the pair $(\pi(a), \pi(a+1))$ is backward.

Proof. We focus on proving the first inequality. The other one can be proven in a similar way. By Lemma 8, the pair $(\pi(b-1), \pi(b))$ is backward. Suppose that $d(\pi(b-1), \pi(b)) \leq d(\pi(a), \pi(a+1)) - 2$. Let $\pi' = \pi[b, a]$. The pairs $(\pi(b-1), \pi(b))$ and $(\pi(a), \pi(a+1))$ are the only pairs of consecutive vertices in the cyclic order that are affected by the reversion. The former is changed to the consecutive pair $(\pi(a+1), \pi(b))$ in π', whose distance is increased by 1; the latter is changed to the consecutive pair $(\pi(a), \pi(b-1))$, whose distance is decreased by 1. As $d(\pi(b-1), \pi(b)) \leq d(\pi(a), \pi(a+1)) - 2$, we conclude that $h(\pi) = h(\pi')$ but $t(\pi')$ is lexicographically smaller than $t(\pi)$. This contradicts our assumption that $t(\pi)$ is lexicographically minimal. □

We now prove the key lemma on our way to determine the hamiltonian spectra of odd cycles.

Lemma 10. *Let n be an odd integer. If $\ell \in \mathcal{H}(C_n)$ and $\ell \geq 2n$, then $\ell - 2 \in \mathcal{H}(C_n)$.*

Proof. Let π be a lexicographically minimal cyclic order among all cyclic orders π' of the vertices of C_n with $h(\pi) = h(\pi') = \ell$. If $t_{\max}(\pi) \leq 2$, then $h(\pi) \leq 2n$ and $h(\pi) = 2n$ by the assumption of the lemma. Consequently, $d(\pi(i), \pi(i+1)) = 2$ for every $i = 1, \ldots, n$, all the pairs $(\pi(i), \pi(i+1))$ are either forward or backward, and $\ell - 2 \in \mathcal{H}(C_n)$ by Lemma 8. Hence, we can assume in the rest that $t_{\max}(\pi) \geq 3$.

We say that a pair $(\pi(i), \pi(i+1))$ of vertices of C_n is *strongly long* if it is long and in addition the following holds:

- the pair $(\pi(i), \pi(i+1))$ is forward, and both the pairs $(\pi(i'-1), \pi(i'))$ and $(\pi(i''), \pi(i''+1))$ are long where i' and i'' are such indices that $\pi(i') = \pi(i) + 1$ and $\pi(i'') = \pi(i+1) - 1$, or
- the pair $(\pi(i), \pi(i+1))$ is backward, and both the pairs $(\pi(i'-1), \pi(i'))$ and $(\pi(i''), \pi(i''+1))$ are long where i' and i'' are such indices that $\pi(i') = \pi(i) - 1$ and $\pi(i'') = \pi(i+1) + 1$.

If every long pair is strongly long, then all the pairs are long: if the forward pair $(v_1, v_{t_{\max}(\pi)+1})$ is strongly long, then the pair $(\pi(\pi^{-1}(v_2) - 1), v_2)$ is backward by Lemma 8 and it is long (the pair $(v_1, v_{t_{\max}(\pi)+1})$ is strongly long). Hence, it must hold that $\pi(\pi^{-1}(v_2) - 1) = v_{t_{\max}(\pi)+2}$. Since this pair is long, it is also strongly long by our assumption. Similarly, one can infer that the pair $(v_3, v_{t_{\max}(\pi)+3})$ is forward, long and thus strongly long. The pair $(v_{t_{\max}(\pi)+4}, v_4)$ is backward and strongly long, etc. After going once along the cycle, we conclude that the pair $(v_{t_{\max}(\pi)+1}, v_1)$ is backward that contradicts our original assumption that it is forward. We conclude that there must exist a pair that is long but not strongly long.

Without loss of generality, we assume that $\pi(1) = v_1$, $\pi(2) = v_{t_{\max}(\pi)+1}$, and the pair $(v_1, v_{t_{\max}(\pi)+1})$ is forward and long but not strongly long. By symmetry, we assume that for i such that $\pi(i) = v_2$, the pair $(\pi(i-1), \pi(i))$ is not long. By Lemma 9, $d(\pi(i-1), \pi(i)) = t_{\max}(\pi) - 1 \geq 2$. Since the pair $(\pi(i-1), \pi(i))$ is backward by Lemma 8, it must hold that $\pi(i-1) = t_{\max}(\pi) + 1$ and thus $i = 3$.

Let s be the largest integer such that the following is true: if $i = 2q \leq s$, then $\pi(i) = v_{t_{\max}(\pi)+2-q}$, and if $i = 2q + 1 \leq s$, then $\pi(i) = v_q$. By our assumption, $s \geq 3$. Observe that $d(\pi(i), \pi(i+1)) = t_{\max}(\pi) + 1 - i$ for every $i = 1, \ldots, s-1$. We now distinguish two cases. The first case is that $s = t_{\max}(\pi) + 1 \geq 4$. In this case, it is straightforward to verify that $h(\pi[s-2, s-1]) = h(\pi) - 2$ and the lemma readily follows.

The other case is that $s \leq t_{\max}(\pi)$. Note that it holds that $d(\pi(s-1), \pi(s)) \geq 2$. Assume that the pair $(\pi(s-1), \pi(s))$ is backward (the other case is symmetric). By our assumptions, the pair $(\pi(s-2), \pi(s-1))$ is forward.

Let i_1 be the index such that $\pi(i_1) = \pi(s-1) - 1$. By Lemma 8, the pair $(\pi(i_1 - 1), \pi(i_1))$ is forward and the pair $(\pi(i_1), \pi(i_1 + 1))$ is backward. By Lemma 9,

$$d(\pi(i_1 - 1), \pi(i_1)) \geq d(\pi(s-1), \pi(s)) - 1 .$$

However, if $d(\pi(i_1 - 1), \pi(i_1)) = d(\pi(s-1), \pi(s)) - 1$, then $\pi(s) = \pi(i_1 - 1)$ that is impossible by our choice of s. Therefore,

$$d(\pi(i_1 - 1), \pi(i_1)) \geq d(\pi(s-1), \pi(s)) = d(\pi(i_1), \pi(s-2)) \geq 2 .$$

On the other hand, by Lemma 9, it also holds the following:

$$d(\pi(i_1), \pi(i_1 + 1)) \geq d(\pi(s-2), \pi(s-1)) - 1 = d(\pi(i_1), \pi(s-2)) \geq 2 .$$

Let i_2 be the index such that $\pi(i_2) = \pi(i_1) - 1 = \pi(s-1) - 2$. By Lemma 8, the pair $(\pi(i_2 - 1), \pi(i_2))$ is forward and the pair $(\pi(i_2), \pi(i_2 + 1))$ is backward. Similarly as above, one can infer the following from Lemma 9:

$$\begin{array}{ll} d(\pi(i_2 - 1), \pi(i_2)) \geq d(\pi(i_1), \pi(i_1 + 1)) - 1 \geq d(\pi(i_2), \pi(s-2)) \geq 2 & \text{and} \\ d(\pi(i_2), \pi(i_2 + 1)) \geq d(\pi(i_1 - 1), \pi(i_1)) - 1 \geq d(\pi(i_2), \pi(s-2)) \geq 2 & . \end{array}$$

Choose now $i_3 = \pi(i_2) - 2 = \pi(s-1) - 3$ and repeat the argument. Continue until $i_k = \pi(s) + 1$. However, both the pairs $(\pi(s-1), \pi(s))$ and $(\pi(i_k), \pi(i_k + 1))$ are backward and $d(\pi(i_k), \pi(i_k + 1)) \geq 2$. Then, $\ell - 2 \in \mathcal{H}(C_n)$ by Lemma 8. □

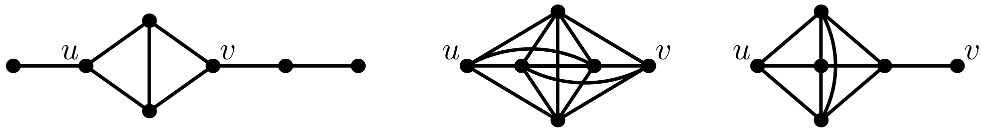
An almost immediate consequence of the previous lemma is the following:

Lemma 11. *For every $k \geq 1$, the hamiltonian spectrum of C_{2k+1} contains all the integers between $4k$ and $k(2k+1) - 2$.*

Proof. Consider the following cyclic order π of the vertices of C_{2k+1}:

$$\pi(i) = \begin{cases} v_{2k-1} & \text{if } i = 2, \\ v_{k-2} & \text{if } i = 3, \\ v_{2k} & \text{if } i = 4, \\ v_{k-1} & \text{if } i = 5, \text{ and} \\ v_{ik \bmod (2k+1)} & \text{otherwise.} \end{cases}$$

It is straightforward to verify that $h(\pi) = k(2k+1) - 3$. In particular, $k(2k+1) - 3 \in \mathcal{H}(C_{2k+1})$. Since $h^+(C_{2k+1}) = k(2k+1)$, we have also that $k(2k+1) \in \mathcal{H}(C_{2k+1})$. The statement of the lemma now follows from Lemma 10. □



$G_{7,5}$ $G_{6,2}$ $G_{6,3}$

Figure 1: Examples of graphs $G_{n,d}$.

We are now ready to finish the case of odd cycles:

Theorem 12. *If $n \geq 3$ is odd, then the following holds:*

$$\begin{aligned}\mathcal{H}(C_n) &= \{n, n+2, \ldots, 2n-5, 2n-3\} \cup \\ &\quad \{2n-2, 2n-1, \ldots, n^2/2 - n/2 - 2\} \cup \\ &\quad \{n^2/2 - n/2\}.\end{aligned}$$

Proof. By Lemma 6, all the numbers contained in $\mathcal{H}(C_n)$ that are smaller or equal to $2n-3$ are odd. Since a single simple reversion changes the number $h(\pi)$ of a cyclic order by at most two (by Lemma 4), $\mathcal{H}(C_n)$ contains all odd numbers between n and $2n-3$. By Lemma 11, $\mathcal{H}(C_n)$ contains all the numbers between $2n-2$ and $n^2/2 - n/2 - 2$. It also holds that $n^2/2 - n/2 - 1 \notin \mathcal{H}(C_n)$ by Lemma 7, and $h^+(C_n) = n^2/2 - n/2 \in \mathcal{H}(C_n)$. Therefore the hamiltonian spectrum of C_n is of the form described in the statement of the theorem. □

5 Upper Hamiltonian Number and Diameter of a Graph

Suppose $d \geq 2$ and $n \geq d+1$. Let $G_{n,d}$ be the graph obtained from a complete graph of order $n-d+2$ by removing an edge uv, adding a path comprised of $\lfloor d/2 \rfloor - 1$ edges ending at the vertex u and a path comprised of $\lceil d/2 \rceil - 1$ edges ending at the vertex v. The graph $G_{n,d}$ has order n and diameter d. Examples of graphs $G_{n,d}$ for small values of n and d can be found in Figure 1.

Lemma 13. *The upper hamiltonian number of $G_{n,d}$, $n \geq d+1$ and $d \geq 2$, is at most $n + \lceil d^2/2 \rceil - 1$.*

Proof. Fix the integers n and d. Let u' be the other end of the path ending at the vertex u. Consider a cyclic order π of the vertices of $G_{n,d}$ and let P_i be a shortest path between the i-th and $(i+1)$-th vertex with respect to the order π. Let us define $k(E)$ for a set E of edges of $G_{n,d}$ to be the number of edges of E contained in the paths $P_1, \dots, P_n$ (counting multiplicities). Let V_i, $i = 0, \dots, d$, be the set of the vertices of $G_{n,d}$ whose distance from u is i, let E_i, $i = 1, \dots, d$, be the edges between the vertices V_{i-1} and V_i, and let F be the edges of the clique induced by $V_{\lfloor d/2 \rfloor}$. Since the sets $E_1, \dots, E_d$ and F form a decomposition of the edge-set of $G_{n,d}$, we have the following equality:

$$h(\pi) = k(E_1) + \cdots + k(E_d) + k(F) \tag{3}$$

Next, we bound the terms in the sum (3).

Since each E_i forms an edge-cut of $G_{n,d}$ and each vertex is the end-vertex of at most two of the paths P_i, the number $k(E_i)$ does not exceed twice the order of the smaller component of $G_{n,d} \setminus E_i$. Hence, the following inequality holds:

$$k(E_i) \le \begin{cases} 2i & \text{if } i \le \lfloor d/2 \rfloor, \\ 2d - 2i + 2 & \text{otherwise.} \end{cases} \tag{4}$$

Finally, we bound $k(F)$. The vertices of $V_{\lfloor d/2 \rfloor}$ induce a clique of order $n - d$ in $G_{n,d}$. An edge of F is contained in a path P_i only if the path P_i joins two vertices of $V_{\lfloor d/2 \rfloor}$. Since the union of the paths P_i form a closed walk visiting every vertex of $G_{n,d}$ at least once and each vertex is an end-vertex of precisely two paths P_i, the number of the paths P_i joining two vertices of $V_{\lfloor d/2 \rfloor}$ does not exceed $n - d - 1$ and thus $k(F) \le n - d - 1$. We now plug (4) and the upper bound on $k(F)$ to (3):

$$\begin{aligned} h(\pi) &= k(E_1) + \cdots + k(E_d) + k(F) \\ &\le 2 + \cdots + 2\lfloor d/2 \rfloor + 2 + \cdots + 2\lceil d/2 \rceil + n - d - 1 \\ &= \lfloor d/2 \rfloor(\lfloor d/2 \rfloor + 1) + \lceil d/2 \rceil(\lceil d/2 \rceil + 1) + n - d - 1 \\ &= \lfloor d/2 \rfloor^2 + \lceil d/2 \rceil^2 + n - 1 = n + \lceil d^2/2 \rceil - 1 \,. \end{aligned}$$

Since the choice of the cyclic order π was arbitrary, the upper hamiltonian number of $G_{n,d}$ does not exceed $n + \lceil d^2/2 \rceil - 1$. □

We are now ready to prove our lower bound on the upper hamiltonian number of a graph in terms of its order and its diameter and show that it is tight:

Theorem 14. *If G is a connected graph of order n and diameter d, $1 \le d \le n-1$, then the upper hamiltonian number $h^+(G)$ is at least $n + \lceil d^2/2 \rceil - 1$. Moreover, for every pair n and d, $1 \le d \le n-1$, there exists a graph G of order n and diameter d for which the equality holds.*

Proof. The existence of graphs that witness the tightness of the bounds on the upper hamiltonian number follows from Lemma 13 for $d \ge 2$. If $d = 1$, the bound is attained for complete graphs. We focus on proving the lower bound in the rest. Consider a graph G of order n and diameter d. Let v_0 be a peripheral vertex of G, i.e., a vertex such that there exists a vertex at distance d from v_0 in G.

Let V_i be the set of the vertices of G at distance i from the vertex v_0 for $i = 1, \ldots, d$, and let v_i be any vertex contained in V_i. Consider the following cyclic order π of the vertices of G:

$$w_1 = v_0, w_2 = v_d, w_3 = v_1, w_4 = v_{d-1}, \ldots, w_{d-1} = v_{d/2-1}, w_d = v_{d/2+1},$$

if d is even, and:

$$w_1 = v_0, w_2 = v_d, w_3 = v_1, w_4 = v_{d-1}, \ldots, w_{d-1} = v_{d/2+3/2}, w_d = v_{d/2-1/2},$$

if d is odd. The vertices $w_{d+1}, \ldots, w_n$ are the vertices of G distinct from $w_1, \ldots, w_d$, and they are sorted in the increasing order according to their distance from v_0.

We now show that the number $h(\pi)$ is at least $n + \lceil d^2/2 \rceil - 1$. Observe that if $v \in V_i$ and $v' \in V_j$, then $d(v, v') \ge i$. Therefore, the following inequality holds for all $i = 1, \ldots, d-1$:

$$d(\pi(i), \pi(i+1)) = d(w_i, w_{i+1}) \ge d - i + 1 \tag{5}$$

Since the vertex $v_{\lceil d/2 \rceil}$ is not among the vertices $w_1, \ldots, w_d$ and the vertices $w_{d+1}, \ldots, w_n$ are sorted according to their distance from v_0, the distance between w_1 and w_n is at least $\lceil d/2 \rceil$. Since the distance between any two vertices is at least one, we infer from (5) the following:

$$\begin{aligned} h(\pi) &= \sum_{i=1}^{n} d(w_i, w_{i+1}) \\ &\ge d + (d-1) + \cdots + 2 + n - d + \lceil d/2 \rceil \\ &= n + (d-1) + \cdots + 2 + \lceil d/2 \rceil \\ &= n + \frac{(d+1)(d-2)}{2} + \lceil d/2 \rceil = n + \left\lceil \frac{d^2}{2} \right\rceil - 1 . \end{aligned}$$

The proof of Theorem 14 is now finished. □

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