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THE NUMBER OF NON-ISOMORPHIC HAMILTONIAN CIRCUITS IN AN n -DIMENSIONAL CUBE

BOHDAN ZELINKA

There is the following problem with applications to error-correcting codes and to control mechanisms:

How many non-isomorphic Hamiltonian circuits are there in the 5-cube?

For $n = 2, 3$ and 4 , the n -cube is known to have respectively 1, 1 and 9 non-isomorphic Hamiltonian circuits. For $n = 5$ bounds have been obtained by E. N. Gilbert [3]. H. L. Abbott [1] and W. H. Mills [5] have contributed to the problem for a general n and the lower and upper bounds $(\sqrt{7})^{2n}$ and $(n/2)^{2n}$ are known. L. Moser conjectured that the correct asymptotic result is $(n/e)^{2n}$. His conjecture is quoted in [4], where the above mentioned problem is referred to as an unsolved one.

Two Hamiltonian circuits in a graph G are called isomorphic, if and only if there exists an automorphism of G which maps one of them onto the other. This a restriction of the usual sense of the concept of isomorphism. In the usual sense obviously any two Hamiltonian circuits of the same graph are isomorphic, because they have equal lengths.

The graph of the n -dimensional cube (or shortly the n -dimensional cube, or more shortly the n -cube), where n is a positive integer, is the undirected graph whose vertices are all possible n -dimensional vectors whose co-ordinates are zeroes and ones and in which two vertices $(a_1, \dots, a_n), (b_1, \dots, b_n)$ are joined by an edge if and only if $a_i \neq b_i$ exactly for one $i, 1 \leq i \leq n$.

In this paper we shall not solve the above problem, but we shall show how this problem can be transferred to a problem of finding the number of words of some formal language. Even after this transfer the solution seems to be a difficult job, even for a computer and even for $n = 5$. But maybe some way for further research will be shown by the results of this paper.

First we shall define the formal languages L_n, L'_n, L''_n .

The alphabet of all three languages L_n, L'_n, L''_n is $A_n = \{1, 2, \dots, n\}$.

A word w over this alphabet belongs to L_n , if and only if the following conditions are satisfied:

- (i) the length of w is 2^n ;

- (ii) any symbol of the alphabet A_n appears in w an even number of times;
- (iii) for each non-empty proper subword of w there exists at least one

symbol of A_n which appears in it an odd number of times.

A word w over the alphabet A_n belongs to L'_n , if and only if it belongs to L_n and satisfies the following condition:

- (iv) if $w = a_1 a_2 \dots a_{2^n}$, then $a_1 < a_{2^n}$.

A word w over the alphabet A_n belongs to L''_n , if and only if it belongs to L'_n and satisfies the following condition (strengthening of (iv)):

- (v) if $w = a_1 a_2 \dots a_{2^n}$ and $a_i = k$ for $k \in A_n$ and $1 \leq i \leq 2^n$, then for any $l \in A_n$, $l < k$, there exists $j < i$ such that $a_j = l$.

In the inequalities the symbols of A_n are taken as numbers in their natural ordering.

If $w = a_1 a_2 \dots a_{2^n}$ is a word over the alphabet A_n , denote by \bar{w} the word w written in the inverse ordering of symbols. If w, w' are two words of the length 2^n , we say that w' is obtained from w by a cyclic permutation, if and only if $w = a_1 \dots a_{2^n}$, $w' = b_1 \dots b_{2^n}$, $b_i = a_{i+k}$ for some fixed k and $i = 1, \dots, 2^n$, the subscript $i + k$ being taken modulo 2^n .

Lemma 1. *Let w be a word of L_n , let w' be a word obtained from w by a cyclic permutation. Then $w' \in L_n$.*

Proof. Any cyclic permutation of the set $\{1, 2, \dots, 2^n\}$ is a power of the cyclic permutation which maps i onto $i + 1$ for $i = 1, \dots, 2^n - 1$ and 2^n onto 1. Therefore it suffices to prove that if the word $w = a_1 a_2 \dots a_{2^n} \in L_n$, then also the word $w'' = a_2 a_3 \dots a_{2^n} a_1 \in L_n$, where $a_i \in A_n$ for $i = 1, \dots, 2^n$. The word w'' is evidently also a word on the alphabet A_n and its length is 2^n . The number of occurrences of any symbol of A_n in w'' is evidently the same as in w , therefore it is also even. Any non-empty proper subword of w'' not containing a_1 is also a nonempty proper subword of w , therefore at least one symbol of A_n occurs in it an odd number of times. The subword a_1 contains a_1 exactly once. Therefore it remains to investigate the subwords of the form $a_j a_{j+1} \dots a_{2^n} a_1$, where $3 \leq j \leq 2^n$. If each symbol of A_n occurs in it an even number of times, then the same holds also for the word $a_2 a_3 \dots a_{j-1}$, because these two subwords form together whole w'' . But $a_2 a_3 \dots a_{j-1}$ is a non-empty proper subword of w , which is a contradiction. Therefore $w'' \in L_n$.

Lemma 2. *Let $w \in L_n$. Then either $w \in L'_n$, or $\bar{w} \in L'_n$.*

Proof. Let $w = a_1 a_2 \dots a_{2^n}$. If $a_1 < a_{2^n}$, then $w \in L'_n$. If $a_1 > a_{2^n}$, then $\bar{w} \in L'_n$. It remains to prove that the case $a_1 = a_{2^n}$ cannot occur. Let us take the word $w'' = a_2 a_3 \dots a_{2^n} a_1$; according to Lemma 1 $w'' \in L_n$. The word $a_{2^n} a_1$ is a non-empty proper subword of w'' ; if $a_{2^n} = a_1$, then in this word

one symbol of A_n would occur twice and other symbols would not occur in it and (iii) would not hold for w'' , which would be a contradiction.

Two words $w = a_1 a_2 \dots a_{2^n}$, $w' = b_1 b_2 \dots b_{2^n}$ over the alphabet A_n are called isomorphic, if and only if for any i and j of the numbers $1, 2, \dots, 2^n$ the equality $a_i = a_j$ is equivalent to $b_i = b_j$.

Lemma 3. *Any two different words from L_n'' are non-isomorphic.*

Proof. Let $w = a_1 a_2 \dots a_{2^n}$, $w' = b_1 b_2 \dots b_{2^n}$, $w \in L_n''$, $w' \in L_n''$ and let w and w' be isomorphic. We shall use induction. According to (v) $a_1 = b_1 = 1$. Now suppose that $a_1 \dots a_i = b_1 \dots b_i$ for some i . If b_{i+1} is equal to some b_j for $j \leq i$, then also a_{i+1} is equal to a_j . As, according to the assumption, $b_j = a_j$, also $b_{i+1} = a_{i+1}$ and $a_1 \dots a_{i+1} = b_1 \dots b_{i+1}$. If b_{i+1} is different from all b_j for $j \leq i$, then according to (v) it is the least of the numbers $1, \dots, n$ which does not occur in $b_1 \dots b_i$. The symbol a_{i+1} must be also different from all a_j for $j \leq i$ and it is the least of the numbers $1, \dots, n$ which does not occur in $a_1 \dots a_i$. Therefore we have proved $w = w'$.

Lemma 4. *Any word of L_n is isomorphic with some word of L_n'' .*

Proof. Let $w = a_1 a_2 \dots a_{2^n}$ be a word of L_n . For $j = 1, \dots, n$ let $l(j)$ be the length of the maximal initial subword of w in which less than j pairwise different symbols occur. Now put $b_{l(j)+1} = j$ for $j = 1, \dots, n$ and for each i such that $1 \leq i \leq 2^n$ and $i \neq l(j) + 1$ for all j put $b_i = j$ if and only if $a_i = a_{l(j)+1}$. From the definition of $l(j)$ it is evident that the symbols $a_{l(j)+1}$ for different j are different, therefore all symbols $1, \dots, n$ occur among them; thus for any $i = 1, \dots, 2^n$ exactly one $j \in A_n$ exists such that $a_i = a_{l(j)+1}$. Now let $a_i = a_k$ for some i and k . This element is equal to some $a_{l(j)+1}$ and therefore $b_i = b_k = j$. On the other hand if $b_i = b_k$, let $b_i = b_k = j$. Then $a_i = a_{l(j)+1}$, $a_k = a_{l(j)+1}$ and therefore $a_i = a_k$. We have proved that w and $w' = b_1 b_2 \dots b_{2^n}$ are isomorphic. It remains to prove that $w' \in L_n''$. Its length is 2^n , therefore (1) is satisfied. (ii) and (iii) follow from the isomorphism of w and w' . Now if $b_i = j$ for some i, j , $1 \leq i \leq 2^n$, $1 \leq j \leq n$, this means that $a_i = a_{l(j)+1}$. For any $k < l$ the symbol $b_{l(k)+1} = k$ and evidently it precedes $b_{l(j)+1}$, because $l(k) < l(j)$ for $k < j$. In the subword $b_1 \dots b_{l(j)}$ only $j - 1$ different symbols of A_n occur; from the above mentioned it follows that they are $1, \dots, j - 1$, therefore if $b_i = j$, then $i \geq l(j) + 1$ and, as $b_{l(j)+1}$ is preceded by all the symbols $1, \dots, j - 1$, so is b_i . Thus $w' \in L_n''$.

Now we shall return to the n -dimensional cube Q_n . We remember some well-known results on its automorphism group [2]. Let \mathfrak{G}_n be the automorphism group of the n -dimensional cube. The order of \mathfrak{G}_n is $2^n \cdot n!$. Now let \mathfrak{F}_n be the subgroup of \mathfrak{G}_n of the order 2^n which is a direct product of n subgroups of the order 2 each of which being generated by an element f_i ($i = 1, \dots, n$)

defined so that if $(a_1, \dots, a_n), (b_1, \dots, b_n)$ are vertices of Q_n and $f_i(a_1, \dots, a_n) = (b_1, \dots, b_n)$, then $b_1 = 1 - a_1, b_j = a_j$ for $j \neq i, 1 \leq j \leq n$. Further let \mathfrak{H}_n be the subgroup of \mathfrak{G}_n of the order $n!$ which consists of all elements h_π , where π is a permutation of the set $\{1, \dots, n\}$, defined so that for any vertex (a_1, \dots, a_n) of Q_n we have $h_\pi(a_1, \dots, a_n) = (a_{\pi(1)}, \dots, a_{\pi(n)})$. Each element of \mathfrak{G}_n is a product of an element of \mathfrak{F}_n with an element of \mathfrak{H}_n .

Now for $i = 1, \dots, n$ by \mathbf{v}_i we denote the n -dimensional vector whose i -th coordinate is 1 and all other coordinates are equal to 0. Two vertices of Q_n (taken as vectors) are joined by an edge if and only if their difference modulo 2 is some \mathbf{v}_i for $i = 1, \dots, n$. Therefore the set of edges of Q_n can be decomposed into classes M_1, \dots, M_n such that the class M_i is the set of all edges for which the difference modulo 2 of the terminal vertices is \mathbf{v}_i .

To any Hamiltonian circuit C of Q_n we assign the word $w(C)$ in the following manner. We go round C starting at the vertex $(0, 0, \dots, 0)$ and that of the two edges incident with it which belongs to M_i with smaller i . After crossing an edge of M_i we write the symbol i . The obtained word is denoted by $w(C)$ and evidently it is in L_n .

Lemma 5. *Let C_1, C_2 be two Hamiltonian circuits of Q_n . Then the following two assertions are equivalent:*

- (a) $w(C_1)$ and $\bar{w}(C_2)$ or $w(C_2)$ are isomorphic
- (b) there exists an automorphism from \mathfrak{H}_n which maps C_1 onto C_2 .

Proof. Assume first that there exists some automorphism $h_\pi \in \mathfrak{H}_n$ which maps C_1 onto C_2 . Let e be an edge of Q_n which belongs to M_i . This means that its terminal vertices are $(a_1, \dots, a_n), (b_1, \dots, b_n)$, where $b_i = 1 - a_i, b_j = a_j$ for $j \neq i$. We have $h_\pi(a_1, \dots, a_n) = (a_{\pi(1)}, \dots, a_{\pi(n)}) = (a'_1, \dots, a'_n), h_\pi(b_1, \dots, b_n) = (b_{\pi(1)}, \dots, b_{\pi(n)}) = (b'_1, \dots, b'_n)$. If $k = \pi^{-1}(i)$ then $b'_k = 1 - a'_k, b'_j = a'_j$ for $j \neq k$. The edge joining (a'_1, \dots, a'_n) and (b'_1, \dots, b'_n) belongs to $M_k = M_{\pi^{-1}(i)}$. We have proved that h_π maps any edge of M_i onto an edge of $M_{\pi^{-1}(i)}$ and therefore it maps two edges belonging to the same class onto two edges belonging again to the same class and two edges belonging to different classes again onto two edges belonging to different classes. Further the vertex $(0, 0, \dots, 0)$ remains fixed in all automorphisms of \mathfrak{H}_n . Therefore if in $w(C_1)$ we substitute $\pi^{-1}(i)$ for i , we obtain either $w(C_2)$ (if the first symbol is less than the last), or $\bar{w}(C_2)$ (otherwise).

Now let $w(C_1), w(C_2)$ be isomorphic. Then there exists a permutation π of $\{1, \dots, n\}$ such that if $w(C_1) = a_1 \dots a_n, w(C_2) = b_1 \dots b_n$, then $b_i = \pi^{-1}(a_i)$ for $i = 1, \dots, n$. The k -th vertex of C_1 encountered on the described journey is $\sum_{j=1}^{k-1} \mathbf{u}_j$, where $\mathbf{u}_j = \mathbf{v}_i$, if the j -th edge of C_1 belongs to M_i .

The k -th vertex of C_2 met on the described journey is $\sum_{j=1}^{k-1} \mathbf{u}_{\pi(j)}$, which is the image of $\sum_{j=1}^{k-1} \mathbf{u}_j$ in h_π . If $w(C_1)$ and $\bar{w}(C_2)$ are isomorphic, the proof is analogous.

Lemma 6. *The following two assertions are equivalent:*

- (a) *the word $w(C_2)$ or $\bar{w}(C_2)$ is obtained from $w(C_1)$ by a cyclic permutation;*
- (b) *there exists an automorphism from \mathfrak{F}_n which maps C_1 onto C_2 .*

Proof. Let there exist a mapping $f \in \mathfrak{F}_n$ which maps C_1 onto C_2 . Then the edge joining two vertices $(a_1, \dots, a_n), (b_1, \dots, b_n)$ belongs to the same class as the edge joining $f(a_1, \dots, a_n), f(b_1, \dots, b_n)$, because the difference modulo 2 of two vertices is preserved by each f_i and therefore also by an arbitrary superposition of these mappings. Therefore if we start from the image of $(0, 0, \dots, 0)$ in f instead of $(0, 0, \dots, 0)$ itself and go according to the word $w(C_1)$, we pass through C_2 and therefore either $w(C_2)$, or $\bar{w}(C_2)$ is obtained from $w(C_1)$ by a cyclic permutation.

Now conversely let $w(C_2)$ be obtained from $w(C_1)$ by a cyclic permutation so that $w(C_1) = a_1 \dots a_{2^n}$, $w(C_2) = b_1 \dots b_{2^n}$, $b_i = a_{i+k}$ for some fixed k . Consider the word $a_1 \dots a_k$ (an initial subword of $w(C_1)$ of the length k)

and take the mapping $f = \prod_{i=1}^k f_{a_i} \in \mathfrak{F}_n$. The l -th vertex, of C_2 is $\sum_{j=1}^{l-1} u_j$, where $u_j = v_i$, if the j -th edge of C_2 belongs to M_i ; in other words if $b_j = i$. The $(k+l)$ -th vertex of C_1 is $\sum_{j=1}^{k+l-1} u'_j = \sum_{j=1}^k u'_j + \sum_{j=k+1}^{k+l-1} u'_j$, where $u'_j = v_i$ if the j -th

edge of C_1 belongs to M_i , in other words if $a_j = i$. But $\sum_{j=1}^k u_j = f(0, 0, \dots, 0)$,

$\sum_{j=k+1}^{k+l-1} u'_j = \sum_{j=1}^{l-1} u_j$, because $b_i = a_{i+k}$ and therefore $u_j = u'_{j+k}$. Thus the $(k+l)$ -th vertex of C_1 is the sum of $f(0, 0, \dots, 0)$ and the l -th vertex of C_2 ; the sum $k+l$ can be here taken modulo 2^n . From the definition of \mathfrak{F}_n we can easily deduce that $f(a_1, a_2, \dots, a_n) = f(0, 0, \dots, 0) + (a_1, a_2, \dots, a_n)$ for any $f \in \mathfrak{F}_n$ and any vertex (a_1, a_2, \dots, a_n) of Q_n . Therefore $f(C_2) = C_1$. If $w(C_1)$ and $\bar{w}(C_2)$ are isomorphic, the proof is analogous. All sums of vectors were taken modulo 2 in this proof.

Now let ρ be a binary relation on L_n'' such that $(w, w') \in \rho$, if either w' , or \bar{w}' is isomorphic to some word obtained from w by a cyclic permutation. It is easy to prove that ρ is an equivalence. From the above proved lemmas a theorem follows.

Theorem. *The number of non-isomorphic Hamiltonian circuits in an n -dimensional cube is equal to the number of equivalence classes of the equivalence ρ on L_n'' .*

Thus we have obtained a method for finding this number. We generate L_n'' and the relation ϱ on it and compute the number of equivalence classes of ϱ .

Finally we shall set a problem. A solution of this problem would make this procedure easier.

Problem. Find a sublanguage L_n''' of L_n'' such that

(a) if $w \in L_n'''$, $w' \in L_n'''$, $w \neq w'$, then neither w' , nor \bar{w}' is isomorphic to a word obtained from w by a cyclic permutation;

(b) for any $w'' \in L_n''$ there exists some $w''' \in L_n'''$ such that either w'' , or \bar{w}'' is isomorphic to a word obtained from w''' by a cyclic permutation;

(c) L_n''' can be characterized by a simple condition (vi) added to (i)–(v).

If such a language were obtained, then the required number of non-isomorphic Hamiltonian circuits in an n -dimensional cube would be equal to the number of elements of L_n''' .

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