A remark on the unitary group of a tensor product of *n* finite-dimensional Hilbert spaces

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Abstract. Let H_i , $1 \le i \le n$ be complex finite-dimensional Hilbert spaces of dimension d_i , $1 \le i \le n$ respectively with $d_i \ge 2$ for every *i*. By using the method of quantum circuits in the theory of quantum computing as outlined in Nielsen and Chuang [2] and using a key lemma of Jaikumar [1] we show that every unitary operator on the tensor product $H = H_1 \otimes H_2 \otimes \ldots \otimes H_n$ can be expressed as a composition of a finite number of unitary operators living on pair product $H_i \otimes H_j$, $1 \le i, j \le n$. An estimate of the number of operators appearing in such a composition is obtained.

Keywords. n-qubit quantum computer; qubits; gates; controlled gates.

1. Introduction

From the theory of quantum computing and quantum circuits (as outlined, for example, in [2]) it is now well-known that every unitary operator on the *n*-fold tensor product $(\mathbb{C}^2)^{\otimes^n}$ of copies of the two-dimensional Hilbert space \mathbb{C}^2 can be expressed as a composition of a finite number of unitary operators living on pair products $H_i \otimes H_j$ where H_i and H_j denote the *i*th and *j*th copies of \mathbb{C}^2 . The proof outlined in [2] also yields an upperbound on the number of such 'pair product' operators as a function of *n*. Following more or less their lines of proof and using a key lemma suggested to me by Jaikumar we present a generalization when copies of \mathbb{C}^2 are replaced by arbitrary finite-dimensional complex Hilbert spaces. Thus the present note is of a pedagogical and expositary nature.

2. The main theorem

Let H_i , $1 \le i \le n$ be complex finite-dimensional Hilbert spaces with dim $H_i = d_i \ge 2$ for every *i*. Let

$$H = H_1 \otimes H_2 \otimes \dots \otimes H_n. \tag{2.1}$$

We shall identify H_i with $L^2(\mathbf{Z}_{d_i})$ where \mathbf{Z}_{d_i} is the additive Abelian group $\{0, 1, 2, ..., d_i - 1\}$ with addition modulo d_i , denoted by \oplus . For any $x \in \mathbf{Z}_{d_i}$ we denote

$$|x\rangle = 1_{\{x\}}$$

Dedicated to Prof. A.K. Roy on his 62nd birthday.

where the right-hand side is the indicator function of the singleton set $\{x\}$ in \mathbb{Z}_{d_i} . Thus $|x\rangle$ is a ket vector in H_i and $\{|x\rangle, x \in \mathbb{Z}_{d_i}\}$ is an orthonormal basis for H_i . For $\underline{x} = (x_1, x_2, \ldots, x_n), x_i \in \mathbb{Z}_{d_i}$ we write $|\underline{x}\rangle = |x_1\rangle|x_2\rangle \ldots |x_n\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_n\rangle$ for the product vector in Dirac notation. Then $\{|\underline{x}\rangle, x_i \in \mathbb{Z}_{d_i}, 1 \le i \le n\}$ is an orthonormal basis for H as defined in (2.1).

A unitary operator U on H is called an (i, j)-gate for some $1 \le i < j \le n$ if it satisfies

$$U|x_1, x_2 \dots zx_n\rangle = \sum_{y \in \mathbb{Z}_{d_i, z \in \mathbb{Z}_{d_j}}} u(x_i, x_j, y, z)|x_1, x_2 \dots x_{i-1}\rangle|y|$$
$$|x_{i+1}x_{i+2} \dots x_{j-1}\rangle|z\rangle|x_{j+1}x_{j+2} \dots x_n\rangle$$

for some scalars $u(x_i, x_j, y, z)$ depending on x_i, x_j, y, z .

Theorem 1. There exists an integer $D = D(d_1, d_2, ..., d_n)$ such that every unitary operator U on H is a composition of the form

$$U = U_{i_1,j_1}U_{i_2,j_2}\dots U_{i_k,j_k}, \quad k \le D$$

where $U_{i_r i_r}$ is an (i_r, j_r) -gate for each r = 1, 2, ..., k.

We divide the proof into several elementary lemmas and finally obtain an upper bound for D. Our first lemma and its proof are taken from [2] and presented for the reader's convenience. To state it we need a definition.

Let \mathcal{H} be an *N*-dimensional complex Hilbert space with a fixed orthonormal basis $\{e_1, e_2, \ldots, e_N\}$. A unitary operator U in \mathcal{H} is said to be *elementary* with respect to this basis and *rooted* in the pair $\{e_i, e_j\}$ for some $1 \le i < j \le N$ if there exist scalars α, β satisfying $|\alpha|^2 + |\beta|^2 = 1$ and

$$Ue_i = \alpha e_i + \beta e_j,$$

$$Ue_j = -\overline{\beta}e_i + \overline{\alpha}e_j,$$

$$Ue_k = e_k \text{ for every } k \notin \{i, j\}.$$

Lemma 1. Let U be any unitary operator in a complex Hilbert space \mathcal{H} with an orthonormal basis $\{e_1, e_2, \ldots, e_N\}$. Then U can be expressed as

$$U = \lambda U_1 U_2 \dots U_k, \quad k \le \frac{N(N-1)}{2}$$

where λ is a scalar of modulus unity and each U_i is elementary with respect to the basis $\{e_1, e_2, \ldots, e_N\}$.

Proof. Let the matrix of U in the basis $\{e_1, e_2, \ldots, e_N\}$, denoted by U again, be given by

$$U = \begin{bmatrix} u_{11} & u_{12} & \dots & u_{1N} \\ u_{21} & u_{22} & \dots & u_{2N} \\ \dots & \dots & \dots & \dots \\ u_{N1} & u_{N2} & \dots & u_{NN} \end{bmatrix}.$$

If $u_{21} = 0$, do nothing. If $u_{21} \neq 0$, left multiply both sides by

$$U_1 = \begin{bmatrix} \alpha & \beta & 0 \\ -\overline{\beta} & \overline{\alpha} & \\ 0 & I_{N-2} \end{bmatrix}$$

where

$$\alpha = \frac{\overline{u}_{11}}{\sqrt{|u_{11}|^2 + |u_{21}|^2}}, \quad \beta = \frac{\overline{u}_{21}}{\sqrt{|u_{11}|^2 + |u_{21}|^2}}.$$

Then the matrix U_1U assumes the form

$$U_{1}U = \begin{bmatrix} u'_{11} & u'_{12} & \dots & u'_{1N} \\ 0 & u'_{22} & \dots & u'_{2N} \\ u_{31} & u_{32} & \dots & u_{3N} \\ \dots & \dots & \dots & \dots \\ u_{N1} & u_{N2} & \dots & u_{NN} \end{bmatrix}.$$

We now repeat the same procedure with left multiplication by a U_2 which is elementary and rooted in $\{e_1, e_3\}$ and make the 31 entry in U_2U_1U vanish. Continuing this N - 1times we get

$$U_{N-1}U_{N-2}\dots U_2U_1U = \begin{bmatrix} v_{11} & v_{12} & \dots & v_{1N} \\ 0 & v_{22} & \dots & v_{2N} \\ 0 & v_{32} & \dots & v_{3N} \\ \vdots & \vdots & & \vdots \\ 0 & v_{N2} & \dots & v_{NN} \end{bmatrix}.$$

The orthonormality of the column vectors on the right-hand side implies $|v_{11}| = 1$, $v_{12} = v_{13} = \cdots = v_{1N} = 0$. Thus

$$\overline{v}_{11}U_{N-1}U_{N-2}\dots U_2U_1U = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & w_{22} & \dots & w_{2N} \\ \vdots & \vdots & & \vdots \\ 0 & w_{N2} & \dots & w_{NN} \end{bmatrix}.$$

Now an induction on the size of the matrix and pooling of the scalars shows the existence of a scalar λ and elementary unitary matrices U_1, U_2, \ldots, U_k such that

$$\overline{\lambda}U_kU_{k-1}\ldots U_1U=I.$$

Transferring the scalar and the U_i 's to the right-hand side gives the required composition with $k \le (N-1) + (N-2) + \dots + 2 + 1 = N(N-1)/2$.

Following the methods of quantum computing we draw a 'circuit diagram' by indicating H_i by a 'wire' and a unitary operator U on $H = H_1 \otimes H_2 \otimes \cdots \otimes H_n$ by

1	
2	-
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<i>n</i> _v	

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and call U a gate. If $u_i \in H_i$ and $|u_1\rangle|u_2\rangle \dots |u_n\rangle \in H$ we say that the gate U produces the *output* $U|u_1\rangle|u_2\rangle \dots |u_n\rangle$ for the *input* $|u_1\rangle|u_2\rangle \dots |u_n\rangle$ and express it as



If we have unitary operators U, V on H then we have

•	U	• •	V	•	=	VU	:

Here an input goes through the first gate U and then through the second gate V. Thus gates must be enumerated from left to right whereas operator multiplication is in the reverse order. If U is a gate on $H_1 \otimes H_2 \otimes \cdots \otimes H_i$ then $U \otimes I$, where I is the identity on $H_{i+1} \otimes \cdots \otimes H_n$ is represented as



This notation can be adapted to any block of wires. We now introduce the most important and central notion of a quantum gate depicted by



This gate denotes the unique unitary operator U in H satisfying for any $\psi \in H_i, a_j \in \mathbb{Z}_{d_i}, j \neq i$

$$U|a_1a_2...a_{i-1}\rangle|\psi\rangle|a_{i+1}a_{i+2}...a_n\rangle$$

= $|a_1a_2...a_{i-1}\rangle(L|\psi\rangle)|a_{i+1}a_{i+2}...a_n\rangle,$
 $U|x_1x_2...x_{i-1}\rangle|\psi\rangle|x_{i+1}x_{i+2}...x_n\rangle$
= $|x_1x_2...x_{i-1}\rangle|\psi\rangle|x_{i+1}x_{i+2}...x_n\rangle$

if

$$(x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n) \neq (a_1, a_2, \ldots, a_{i-1}, a_{i+1}, \ldots, a_n),$$

L being a unitary operator in H_i . It is called a quantum gate *controlled* at $a_1, a_2, \ldots, a_{i-1}$, a_{i+1}, \ldots, a_n on the wires $1, 2, \ldots, i-1, i+1, \ldots, n$ and *targeted* by the unitary operator *L* on the *i*th wire. Denote the set of all such gates by C_{n-1} .

For any of the groups \mathbf{Z}_{d_i} we write for any $x \in \mathbf{Z}_{d_i}$

$$\alpha(x) = \begin{cases} 1 & \text{if } x = 0, \\ 0 & \text{otherwise.} \end{cases}$$

Then we have, for example,



where U is the unique unitary operator in $H_1 \otimes H_2 \otimes H_3$ satisfying

$$U|x_1\rangle|\psi\rangle|x_3\rangle = |x_1\rangle(L^{\alpha(x_1-a_1)\alpha(x_3-a_3)}|\psi\rangle)|x_3\rangle$$

for all $x_1 \in \mathbb{Z}_{d_1}, x_3 \in \mathbb{Z}_{d_3}, \psi \in H_2, a_1 \in \mathbb{Z}_{d_1}, a_2 \in \mathbb{Z}_{d_2}$ and *L* a unitary operator in H_2 .

We denote by C_k the set of all gates which are controlled on k wires and targeted by some unitary operator on a wire different from these k wires. For example



is a C_1 gate satisfying

$$U|x_1x_2\ldots x_n\rangle = |x_1x_2\ldots x_{j-1}\rangle (L^{\alpha(x_i-a_i)}|x_j\rangle)|x_{j+1}x_{j+2}\ldots x_n\rangle$$

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for all $x_r \in \mathbf{Z}_{d_r}$, $1 \le r \le n$.

Whenever the controls are at the null elements of the groups \mathbf{Z}_{d_i} we indicate them by dots on the appropriate wires. For example



is a gate in $H_1 \otimes H_2 \otimes \cdots \otimes H_6$ satisfying

$$U|x_1x_2...x_6\rangle = |x_1x_2\rangle (L^{\alpha(x_2)\alpha(x_5)\alpha(x_6)}|x_3\rangle)|x_4x_5x_6\rangle$$

for all $x_i \in \mathbf{Z}_{d_i}$, $1 \le i \le 6$. This is an example of a C_3 gate which is controlled at 0 on wires 2, 5, 6 and targeted by *L* on wire 3.

We denote by $C_k^0 \subset C_k$ the subset of those gates where all the controls are at 0. C_0 denotes the set of all gates in $H_1 \otimes H_2 \otimes \cdots \otimes H_n$ which are targeted on one wire but without any control on other wires. For example



is a C_0 gate satisfying

$$U|x_1x_2\ldots x_n\rangle = |x_1\ldots x_{i-1}\rangle (L|x_i\rangle)|x_{i+1}\ldots x_n\rangle$$

for all $x_i \in \mathbf{Z}_{d_i}$, $1 \le i \le n$.

When the targeted operator *L* on the *i*th wire is the cyclic permutation of the basis in \mathbb{Z}_{d_i} , i.e., $L|x\rangle = |x \oplus 1\rangle$ we indicate it on the *i*th wire by \oplus . For example,



means the gate satisfying

 $U|x_1x_2x_3\rangle = |x_1x_2\rangle|x_3 \oplus \alpha(x_1 - a_1)\rangle.$

With these conventions adapted to our situation from the theory of quantum computing (as outlined for example in [2,3]) we are ready to formulate and prove a lemma due to Jaikumar [1].

Lemma 2. [1] Let L be any unitary operator in H_n . Then



where $B = C^{-1}$, $C = L^{1/d_{n-1}}$ is a fixed d_{n-1} th root of L. The right-hand side is a composition of $2(d_{n-1}+1)$ gates from C_{n-2}^0 .

Proof. Consider an input $|x_1x_2...x_{n-1}\rangle|\psi\rangle$. The left-hand side produces the output

$$|x_1x_2\dots x_{n-1}\rangle L^{\alpha(x_1)\alpha(x_2)\dots\alpha(x_{n-1})}|\psi\rangle.$$

$$(2.2)$$

We now examine the output produced by the 'quantum circuit' on the right-hand side. After passage through the first C_{n-2}^0 gate we get

$$|x_1x_2\ldots x_{n-1}\rangle L^{\alpha(x_2)\ldots\alpha(x_{n-1})}|\psi\rangle$$

When this passes through the next *j* pairs of gates with $j \leq d_{n-1}$ we get the output

$$|x_1x_2...x_{n-2}\rangle|x_{n-1} \oplus j\alpha(x_1)...\alpha(x_{n-2})\rangle B^{r_j\alpha(x_2)...\alpha(x_{n-2})}L^{\alpha(x_2)...\alpha(x_{n-1})}|\psi\rangle$$

where

$$r_j = \sum_{s=1}^{j} \alpha(x_{n-1} \oplus s\alpha(x_1) \dots \alpha(x_{n-2})).$$

Since d_{n-1} and 0 are to be identified in the group $\mathbf{Z}_{d_{n-1}}$ we see that the passage through the d_{n-1} th pair and then the last gate yields the final output

$$|x_1x_2\dots x_{n-1}\rangle C^{\alpha(x_1)\dots\alpha(x_{n-2})} B^{r\alpha(x_2)\dots\alpha(x_{n-2})} L^{\alpha(x_2)\dots\alpha(x_{n-1})} |\psi\rangle$$
(2.3)

where

$$r = \sum_{s=0}^{d_{n-1}-1} \alpha(x_{n-1} \oplus s\alpha(x_1)\alpha(x_2) \dots \alpha(x_{n-2})).$$
(2.4)

Suppose $x_j \neq 0$ for some $2 \leq j \leq n-2$. Then the expression (2.3) reduces to $|x_1x_2...x_{n-1}\rangle|\psi\rangle$ and coincides with (2.2). Thus it suffices to examine the case when $x_j = 0$ for $2 \leq j \leq n-2$. Then (2.3) and (2.4) reduce respectively to

$$|x_10, 0...0x_{n-1}\rangle C^{\alpha(x_1)} B^r L^{\alpha(x_{n-1})} |\psi\rangle$$
(2.5)

and

$$r = \sum_{s=0}^{d_{n-1}-1} \alpha(x_{n-1} \oplus s\alpha(x_1)).$$
(2.6)

Now we examine four cases.

Case 1. $x_1 \neq 0, x_{n-1} \neq 0$. We have $\alpha(x_1) = \alpha(x_{n-1}) = r = 0$ and (2.5) reduces to $|x_1 0 0 \dots 0 x_{n-1}\rangle |\psi\rangle$.

Case 2. $x_1 \neq 0, x_{n-1} = 0$. We have $\alpha(x_1) = 0, \alpha(x_{n-1}) = 1, r = d_{n-1}$ and (2.5) reduces to

$$|x_100\ldots 0\rangle B^{d_{n-1}}L|\psi\rangle = |x_10\ldots 0\rangle |\psi\rangle,$$

owing to the definition of B and C in the lemma.

Case 3. $x_1 = 0, x_{n-1} \neq 0$.

Now $\alpha(x_1) = 1$, $\alpha(x_{n-1}) = 0$ and $r = \sum_{s=0}^{d_{n-1}-1} \alpha(x_{n-1} \oplus s)$. As *s* varies from 0 to $d_{n-1} - 1$ exactly one of the elements $x_{n-1} \oplus s$ is 0 and hence r = 1. Thus (2.5) reduces to $|00 \dots 0x_{n-1}\rangle CB|\psi\rangle = |00 \dots 0x_{n-1}\rangle|\psi\rangle$.

Case 4. $x_1 = 0, x_{n-1} = 0$.

Now $\alpha(x_1) = 1, \alpha(x_{n-1}) = 1$ and $r = \sum_{s=0}^{d_{n-1}-1} \alpha(s) = 1$. Thus (2.5) reduces to $|00...0\rangle CBL|\psi\rangle = |00...0\rangle L|\psi\rangle$.

In other words, in all the cases, the two circuits on both sides of the lemma produce the same output. The last part of the lemma is obvious. \Box

COROLLARY 1

Let $d = \max_i d_i$. Then any gate in C_{n-1}^0 is a composition of at most $[2(d+1)]^{n-2}$ gates in C_1^0 .

Proof. By the last part of Lemma 3 and a shuffle of the wires it follows that any C_{n-1}^0 gate is a composition of at most 2(d + 1) gates from C_{n-2}^0 . Rest follows from induction.

Lemma 3. In $H_i = L^2(\mathbf{Z}_{d_i})$ denote by $T_a, a \in \mathbf{Z}_{d_i}$ the unitary operator satisfying $T_a|x\rangle = |x + a\rangle$ for every $x \in \mathbf{Z}_{d_i}$. Then for any $a_i \in \mathbf{Z}_{d_i}$, i = 1, 2, ..., n - 1 and any unitary operator L in H_n the following holds:



Proof. Apply both sides to the input $|x_1x_2...x_{n-1}\rangle|\psi\rangle$ for any $x_i \in \mathbb{Z}_{d_i}$, i = 1, 2, ..., n-1 and $\psi \in H_n$. A straightforward check by inspection completes the proof.

Lemma 4. Any C_{n-1} gate can be expressed as a composition of at most 2(n-1) gates from C_0 and $[2(d+1)]^{n-2}$ gates from C_1^0 .

Proof. By Lemma 3 any C_{n-1} gate is a composition of 2(n-1) gates from C_0 and a C_{n-1}^0 gate. The required result follows from Corollary 1.

To state our next lemma we introduce a definition.

For any $a \neq b, a, b \in \mathbb{Z}_{d_i}$ we define the *swap* operator S(a, b) in $L^2(\mathbb{Z}_{d_i})$ as the unique unitary operator satisfying

$$S(a, b)|x\rangle = |x\rangle \text{ if } x \notin \{a, b\},$$
$$= |b\rangle \text{ if } x = a,$$
$$= |a\rangle \text{ if } x = b.$$

Lemma 5. Let $a_i, b_i \in \mathbb{Z}_{d_i}, i = 1, 2, ..., k, a_i \neq b_i$ for every *i*. Consider the unitary operator U in $H_1 \otimes H_2 \otimes \cdots \otimes H_k$ determined by

$$U|a_1a_2...a_k\rangle = \alpha |a_1a_2...a_k\rangle + \beta |b_1b_2...b_k\rangle,$$

$$U|b_1b_2...b_k\rangle = -\overline{\beta} |a_1a_2...a_k\rangle + \overline{\alpha} |b_1b_2...b_k\rangle,$$

$$U|x_1x_2...x_k\rangle = |x_1x_2...x_k\rangle \quad if (x_1, x_2, ..., x_k) \notin \{(a_1, a_2, ..., a_k), (b_1, b_2, ..., b_k)\}$$

where α , β are scalars satisfying $|\alpha|^2 + |\beta|^2 = 1$. Define the unitary operator L in H_k by the equations

$$L|a_k\rangle = \alpha |a_k\rangle + \beta |b_k\rangle,$$

$$L|b_k\rangle = -\overline{\beta} |a_k\rangle + \overline{\alpha} |b_k\rangle,$$

$$L|x\rangle = |x\rangle \quad if x \notin \{a_k, b_k\}$$

Then U can be expressed as



where the circuit has 2k - 1 gates from C_{k-1} and the last (k - 1) gates are also the first (k - 1) gates in reverse order.

Proof. By the definition of *L*, the *k*th gate in the circuit is an elementary operator with respect to the basis $\{|x_1x_2...x_k\rangle, x_i \in \mathbb{Z}_{d_i}, 1 \le i \le k\}$ rooted in the pair $\{|a_1a_2...a_k\rangle, |a_1, a_2...a_{k-1}, b_k\rangle\}$ and all other gates are unitary operators whose squares are equal to identity. Since the composition of the last (k-1) gates is the inverse of the composition of the first (k-1) gates it follows that the circuit in the lemma yields a gate which is conjugate to an elementary operator. Now consider the two inputs $|a_1a_2...a_k\rangle$ and $|b_1b_2...b_k\rangle$ for the circuit in the lemma. By the definition of *L* it follows that the respective outputs are, indeed, $U|a_1a_2...a_k\rangle$ and $U|b_1b_2...b_k\rangle$. Thus *U* is represented by the circuit in the lemma.

Proof of Theorem 1. Let $N = d_1 d_2 \dots d_n$ denote the dimension of $H = H_1 \otimes H_2 \otimes \dots \otimes H_n$ and let $d = \max_i d_i$. Now let U be an arbitrary unitary operator in H. By Lemma 1, Ucan be expressed as a product of a scalar λ of modulus unity and at most N(N - 1)/2unitary operators, each of which is elementary with respect to the basis { $|x_1x_2...x_n\rangle$, $x_i \in \mathbb{Z}_{d_i}$, $1 \le i \le n$ }.

Now consider a pair of product vectors of the form

 $|x_1x_2...x_n\rangle, |y_1y_2...y_n\rangle$ where $\#\{i|x_i = y_i\} = r$.

After an appropriate permutation of $\{1, 2, ..., n\}$ (or equivalently, a shuffling of the wires) we may assume, without loss of generality, that

$$(x_1, x_2, \dots, x_n) = (c_1, c_2, \dots, c_r, a_1, a_2, \dots, a_k),$$

$$(y_1, y_2, \dots, y_n) = (c_1, c_2, \dots, c_r, b_1, b_2, \dots, b_k)$$

where k + r = n and $a_i \neq b_i$ for every $1 \leq i \leq k$. By adding *r* more wires to the circuit in Lemma 5 and putting controls at c_1, c_2, \ldots, c_r on these wires above each of the gates we observe that a gate which is elementary with respect to our fixed coordinate system and rooted in the pair $\{|c_1c_2...c_ra_1a_2...a_k\rangle, |c_1c_2...c_rb_1b_2...b_k\rangle\}$ can be expressed as a composition of (2k - 1) gates from C_{n-1} . Now an application of Lemma 4 shows that this

same elementary operator can be expressed as a composition of at most $(2k-1)\{2(n-1)+[2(d+1)]^{n-2}\}$ gates from $\mathcal{C}_0 \cup \mathcal{C}_1^0$. Thus U can be expressed as a composition of at most

$$\frac{N(N-1)}{2}(2n-1)\{2(n-1)+[2(d+1)]^{n-2}\}$$
(2.7)

gates from $C_0 \cup C_1^0$. Any gate in $C_0 \cup C_1^0$, is, indeed, an (i, j) gate. Choosing D equal to the expression in (2.7) the proof becomes complete.

Remark 1. When $d_i = d$ for every *i* and *n* increases to ∞ the number *D* in Theorem 1 is $O(n[2d^2(d+1)]^n)$.

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