Constructing three-qubit unitary gates in terms of Schmidt rank and CNOT gates

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Abstract
It is known that every two-qubit unitary operation has Schmidt rank one, two or four, and the construction of three-qubit unitary gates in terms of Schmidt rank remains an open problem. We explicitly construct the gates of Schmidt rank from one to seven. It turns out that the three-qubit Toffoli and Fredkin gate, respectively, have Schmidt rank two and four. As an application, we implement the gates using quantum circuits of CNOT gates and local Hadamard and flip gates. In particular, the collective use of three CNOT gates can generate a three-qubit unitary gate of Schmidt rank seven in terms of the known Strassen tensor from multiplicative complexity.

Keywords Schmidt rank · Three-qubit unitary gate · CNOT gate

1 Introduction
The implementation of multiqubit unitary gates is one of the central problems in quantum computing [1–4]. Multiqubit gates can be performed by adiabatic passage with an optical cavity [5] and resource-efficient microwave [6]. The entangling multiqubit gate is key to the realization of quantum error correction by superconducting circuit [7] and geometric phase from quantum measurement [8]. On the other hand, the Schmidt rank plays a key role when determining whether a bipartite unitary operation is a controlled unitary operation [9–11], the decomposition of multipartite unitary gates into...
the product of controlled unitary gates for implementing efficiently quantum circuits [12], and the derivation of entangling power of bipartite unitaries for quantifying how much entanglement they can create locally [13,14].

It has been proved that every two-qubit unitary operation has Schmidt rank one, two or four [15]. For the three-qubit systems, the Schmidt decomposition of any pure three-qubit state has been found [16]. The mixed three-qubit states have also been classified into different entanglement classes [17]. But as far as we know, it is an open problem of characterizing three-qubit unitary operations in terms of Schmidt rank. In this paper, we construct such operations of Schmidt rank from one to seven, respectively. We introduce the preliminary facts on the Schmidt rank of tripartite matrices in Lemma 1 and Corollary 2. Then the open problem can be solved using basic knowledge of linear algebra. This is realized in Theorem 3 by constructing explicit examples. In particular, the unitary operation of Schmidt rank seven is isomorphic to the well-known Strassen tensor from multiplicative complexity [18]. This is also of interest in the field of computational science. Next, we present another three-qubit gate in (11) and prove that it has Schmidt rank at least six but not more than eight in Theorem 4. On the other hand, it turns out that the well-known three-qubit Toffoli and Fredkin gate respectively have Schmidt rank two and four. Then we implement three-qubit unitary gates of Schmidt rank one to seven using controlled-NOT (CNOT) gates and local unitary gates such as the Hadamard gates and qutrit flip gates. We illustrate the implementation in Figs. 1, 2, 3, 4, 5, 6 and 7. In Theorem 5, we show that the combination of two CNOT gates and local unitary gates can generate a three-qubit unitary gate of Schmidt rank one, two or four only. Hence three CNOT gates are necessary for the implementation of gates of Schmidt rank three, five, six and seven. Furthermore, we show in Theorem 6 that the collective use of three CNOT gates can generate a three-qubit unitary gate of Schmidt rank seven in terms of Strassen tensor.

The implementation of quantum gates is usually carried out using CNOT gates assisted with local unitary gates. The efficiency is thus evaluated by the number of CNOT gates involved in the implementation. It has been proved that the theoretical lower bound for the number of CNOT gates needed in simulating an arbitrary $n$-qubit gate is $\lceil \frac{1}{4} (4^n - 3n - 1) \rceil$ [19,20], while the number can be $\lceil \frac{23}{48} 4^n - \frac{3}{2} 2^n + \frac{1}{3} \rceil$ by implementation [21]. Further, a circuit has been constructed for $n$-qubit states by CNOT gates and one-qubit rotations [22]. Besides, at most four CNOT gates are needed to transform any pure three-qubit gates into another pure state [23]. So far there is little study on the connection between the Schmidt rank of a multiqubit gate and the number of required CNOT gates. Our results thus initiate the problem of understanding quantum circuit in terms of Schmidt rank.

The rest of this paper is organized as follows. In Sect. 2, we introduce the preliminary knowledge of this paper. Then we construct three-qubit unitary operations of Schmidt rank one to seven, respectively. We also construct a three-qubit unitary operation of Schmidt rank six or seven or eight. In Sect. 3, we implement three-qubit unitary gates using CNOT gates assisted by local unitary gates. We conclude in Sect. 4.
2 Construction of three-qubit unitary gates

We begin by introducing the notations used in this paper. We refer to $\mathbb{C}^d$ as the $d$-dimensional Hilbert space. We denote $\mathbb{M}_{a \times b}$ as the set of $a \times b$ matrices. In particular, if $a = b$ then we refer to $\mathbb{M}_a$ as the set of $a \times a$ matrices. Let $M^\dagger$ be the transpose and complex conjugate of matrix $M$, i.e., $M^\dagger = (M^T)^*$. Let $I_n$ be the $n \times n$ identity matrix. Further we shall refer to $I_2$, $\sigma_1$, $\sigma_2$ and $\sigma_3$ as the identity matrix and three Pauli matrices, respectively. Further, we denote $S_0$, $S_1$, $S_2$, $S_3$ as the $2 \times 2$ matrices

\[
S_0 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad S_1 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad S_2 = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad S_3 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix},
\]

respectively.\(^1\) We define the Schmidt rank of an $n$-partite matrix $U$ on the $n$-partite Hilbert space $H_1 \otimes ... \otimes H_n := \mathbb{C}^{d_1} \otimes ... \otimes \mathbb{C}^{d_n}$ as the minimum integer $r$ such that $U = \sum_{j=1}^{r} A_{j,1} \otimes ... \otimes A_{j,n-1} \otimes A_{j,n}$ for some $d_i \times d_i$ matrix $A_{j,i}$ and $i = 1, \ldots, n$. If $n = 2$ then the definition reduces to the Schmidt rank of bipartite matrix $U$. For convenience, we refer to $sr(U)$ as the Schmidt rank of $U$. By regarding $U$ as a block matrix, one can effectively derive the Schmidt rank of $U$ by computing the number of its linearly independent matrix blocks. Unfortunately computing the Schmidt rank of a tripartite matrix is an NP-hard problem [24]. Nevertheless, we can construct the relation between bipartite and multipartite matrices, so as to investigate the relation between the Schmidt rank of them. For example, we can regard $U$ as a bipartite unitary matrix $US$ of system $S = \{1, \ldots, k\}$ and $\bar{S} = \{k+1, \ldots, n\}$. By writing the Schmidt decomposition of $US$, i.e., $US = \sum_{i=1}^{r} B_i \otimes C_i$ with $r = sr(US)$, we shall say that the span of $B_1, \ldots, B_r$ is the $S$-space of $U$. Similarly, the span of $C_1, \ldots, C_r$ is the $\bar{S}$-space of $U$. It is straightforward to show the inequality $sr(U) \geq sr(US)$. This is a frequently used lower bound of the Schmidt rank of $U$ because the Schmidt rank of bipartite matrices are known to be computable. We will use the inequality in the paper without explanation unless stated otherwise.

To find a systematic way of deriving the Schmidt rank, we review a fact from Theorem 3.1.1.1 on p68 of [18].

**Lemma 1** Suppose $U = \sum_{j=1}^{r} Q_j \otimes R_j$ is a tripartite matrix where $Q_j$ on $H_A \otimes H_B$ are linearly independent, and $R_j$ on $H_C$ are also linearly independent. Then the Schmidt rank of $U$ is the minimal number of product matrices spanning the space including the space spanned by $Q_1, \ldots, Q_r$.

Then we present a corollary of this lemma.

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\(^1\) Note that one often uses the notations $\sigma_+$ and $\sigma_-$ for $S_1$ and $S_2$; here, we do not use them for the consistency of expressions of the formulas in (1).

\(^2\) The notion is equivalent to the tensor rank in matrix multiplication. We denote it as Schmidt rank because a similar use has been proposed in [29].
Corollary 2 We still use the notations in Lemma 1. Suppose \( sr(U) = n \) and let \( U = \sum_{i=1}^{sr(U)} X_i \otimes Y_i \otimes Z_i \). If \( Q_1, \ldots, Q_n \) are product matrices then we may assume that \( Q_j = X_j \otimes Y_j \) for \( j = 1, \ldots, n \).

Proof We know that \( Q_i \) is the linear combination of \( X_j \otimes Y_j \) for \( j = 1, 2, \ldots, sr(U) \). If \( i = 1 \) and the coefficient of \( X_1 \otimes Y_1 \) is nonzero, then we may express \( X_1 \otimes Y_1 \) as the linear combination of \( Q_1 \) and \( X_2 \otimes Y_2, \ldots, X_{sr(U)} \otimes Y_{sr(U)} \). Using the expression, we obtain that \( X_j \otimes Y_j \) is the linear combination of the same matrices. Hence we may assume that \( Q_1 = X_1 \otimes Y_1 \). One can similarly prove the assertion for \( j = 2, \ldots, n \). \( \square \)

The above corollary plays an important role in constructing three-qubit unitary matrices of Schmidt rank from one to seven, respectively. This is presented in Theorem 3, namely the first main result of this section. Next we construct the three-qubit unitary operation of Schmidt rank six or seven or eight in Theorem 4. This is the second main result of this section. We begin by studying three-qubit unitary matrices of Schmidt rank up to seven.

Theorem 3 The three-qubit unitary operation of Schmidt rank up to seven exists.

Proof Let \( U \) be a three-qubit unitary operation. If suffices to find \( U \) with \( sr(U) = 1, 2, 3, 4, 5, 6 \) and 7, respectively. It is known that the two-qubit unitary \( V \) of Schmidt rank one, two or four exists. So \( U = I_2 \otimes V \) has Schmidt rank one, two or four. Next one can show that \( U_3 = \frac{1}{\sqrt{3}} (I_2^{\otimes 3} + i\sigma_1^{\otimes 3} + i\sigma_3^{\otimes 3}) \) is a three-qubit unitary matrix of Schmidt rank three.

Third we construct \( U = U_5 \) of Schmidt rank five. Let

\[
U_5 = \frac{1}{2} S_0 \otimes (I_2 \otimes I_2 + \sigma_1 \otimes \sigma_1 + \sigma_2 \otimes \sigma_2 + \sigma_3 \otimes \sigma_3)
+ S_3 \otimes I_2 \otimes \sigma_1
= \frac{1}{2} S_0 \otimes I_2 \otimes I_2 + (\frac{1}{2} S_0 \otimes \sigma_1 + S_3 \otimes I_2) \otimes \sigma_1
+ \frac{1}{2} S_0 \otimes \sigma_2 \otimes \sigma_2 + \frac{1}{2} S_0 \otimes \sigma_3 \otimes \sigma_3.
\tag{2}
\]

One can show that \( U_5 \) is unitary, and \( 4 \leq sr(U_5) \leq 5 \). If \( sr(U_5) = 4 \) then \( U_5 = \sum_{j=1}^{4} A_j \otimes B_j \otimes C_j \) with some \( 2 \times 2 \) matrices \( A_j, B_j \) and \( C_j \). By comparing with (2), one can show that \( C_j \)’s are linear independent, namely they span the space of the \( 2 \times 2 \) matrices. So the \( AB \) space of \( U_5 \) is spanned by \( A_j \otimes B_j \)’s, namely four linearly independent product matrices. Using (2), one can show that the \( AB \) space of \( U_5 \) is spanned by the four linearly independent matrices

\[
\frac{1}{2} S_0 \otimes \sigma_1 + S_3 \otimes I_2, \quad S_0 \otimes I_2,
S_0 \otimes \sigma_2, \quad S_0 \otimes \sigma_3.
\tag{3}
\]

Because \( A_j \otimes B_j \)’s and (3) are two bases of the \( AB \) space of \( U_5 \), each \( A_j \otimes B_j \) is the linear combination of the four matrices in (3). So at least one of \( A_j \otimes B_j \)’s is the
linear combination of them such that the coefficient of $\frac{1}{2}S_0 \otimes \sigma_1 + S_3 \otimes I_2$ is nonzero. However one can show that this linear combination is not a product matrix. We have proven that $sr(U_5) \neq 4$. Hence $sr(U_5) = 5$.

Fourth we construct $U = U_6$ of Schmidt rank six. Let

$$U_6 = \frac{1}{2} S_0 \otimes (I_2 \otimes I_2 + \sigma_1 \otimes \sigma_1 + \sigma_2 \otimes \sigma_2 + \sigma_3 \otimes \sigma_3)$$

$$+ \frac{1}{\sqrt{2}} S_3 \otimes (I_2 \otimes \sigma_1 + \sigma_2 \otimes \sigma_3)$$

$$= \frac{1}{2} S_0 \otimes I_2 \otimes I_2 + \frac{1}{2} S_0 \otimes \sigma_1 \otimes \sigma_1$$

$$+ \frac{1}{\sqrt{2}} S_3 \otimes I_2 \otimes \sigma_1 + \frac{1}{2} S_0 \otimes \sigma_2 \otimes \sigma_2$$

$$+ \frac{1}{2} S_0 \otimes \sigma_3 \otimes \sigma_3 + \frac{1}{\sqrt{2}} S_3 \otimes \sigma_2 \otimes \sigma_3. \quad (4)$$

Suppose that $sr(U_6) \leq 5$. We may assume that $U_6 = \sum_{i=1}^5 Q_i \otimes C_i$ with the product matrices $Q_i \in M_2 \otimes M_2$. Using Corollary 2 and (4), we may assume that

$$Q_1 = S_0 \otimes I_2,$$  

$$Q_2 = S_0 \otimes \sigma_2,$$  

$$S_0 \otimes \sigma_1 + \sqrt{2} S_3 \otimes I_2 = \sum_{j=1}^5 a_j Q_j, \quad (7)$$

$$S_0 \otimes \sigma_3 + \sqrt{2} S_3 \otimes \sigma_2 = \sum_{j=1}^5 b_j Q_j, \quad (8)$$

for some complex numbers $a_j$ and $b_j$. Let $Q_j = A_j \otimes B_j$ with $2 \times 2$ matrices $A_j$ and $B_j$ for $j = 3, 4, 5$. Eqs. (7) and (8) imply that $\sigma_1, I_2, \sigma_3, \sigma_2 \in \text{span}\{B_3, B_4, B_5\}$. It is a contradiction with the fact that $\text{span}\{B_3, B_4, B_5\}$ has dimension at most three. We have shown that $sr(U_6) \geq 6$. On the other hand, (4) shows that $sr(U_6) \leq 6$. Hence $sr(U_6) = 6$.

Fifth we construct $U = U_7$ of Schmidt rank seven. Let

$$U_7 = S_1 \otimes S_2 \otimes S_0 + S_2 \otimes S_3 \otimes S_0$$

$$+ S_0 \otimes S_0 \otimes S_1 + S_3 \otimes S_1 \otimes S_1$$

$$+ S_1 \otimes S_1 \otimes S_2 + S_2 \otimes S_0 \otimes S_2$$

$$+ S_0 \otimes S_3 \otimes S_3 + S_3 \otimes S_2 \otimes S_3, \quad (9)$$

One can verify that $U_7$ is unitary. Further, we perform the permutation $(3210)$ on system $A$, $(320)$ on system $B$, and $(13)$ on system $C$ of $U_7$. Then $U_7$ is isomorphic to the known $4 \times 4 \times 4$ Strassen tensor, which has Schmidt rank seven. Hence $sr(U_7) = 7$. We have proven the assertion. \hfill \square
In contrast to the gate of Schmidt rank four constructed in the above proof, one can show that the three-qubit unitary operation in Eq. (18) of the paper [25], written as

\[ U = \frac{1}{\sqrt{2}} (S_0 \otimes I_2 \otimes I_2 + S_1 \otimes \sigma_3 \otimes \sigma_3 + S_2 \otimes \sigma_1 \otimes \sigma_1 + S_3 \otimes \sigma_2 \otimes \sigma_2), \]

has Schmidt rank at most 16. Actually we can express \( U_{123} \) as the sum of 16 product matrices as follows.

\[
U' = \frac{1}{\sqrt{2}} \left( (S_0 \otimes S_0 \otimes S_0 + S_0 \otimes S_1 \otimes S_2 + S_1 \otimes S_2 \otimes S_0 + S_1 \otimes S_3 \otimes S_2) \otimes \begin{bmatrix} 1 & i \\ 0 & 0 \end{bmatrix} \right. \\
+ (S_0 \otimes S_0 \otimes S_1 + S_0 \otimes S_1 \otimes S_3 + S_1 \otimes S_2 \otimes S_1 + S_1 \otimes S_3 \otimes S_3) \otimes \begin{bmatrix} 0 & 0 \\ 1 & i \end{bmatrix} \\
+ (S_2 \otimes S_2 \otimes S_2 - S_2 \otimes S_3 \otimes S_0 - S_3 \otimes S_0 \otimes S_2 + S_3 \otimes S_1 \otimes S_0) \otimes \begin{bmatrix} 0 & 0 \\ 1 & -i \end{bmatrix} \\
+ (S_2 \otimes S_2 \otimes S_3 - S_2 \otimes S_3 \otimes S_1 - S_3 \otimes S_0 \otimes S_3) \\
+ S_3 \otimes S_1 \otimes S_1) \otimes \begin{bmatrix} -1 & i \\ 0 & 0 \end{bmatrix}. \tag{10}
\]

In the following, we construct a three-qubit matrix \( U_8 \) using (1) and show it has Schmidt rank six or seven or eight in Theorem 4. This is the second main result of this section.

\[
U_8 = S_0 \otimes S_0 \otimes S_0 + S_1 \otimes S_3 \otimes S_0 \\
+ S_2 \otimes S_0 \otimes S_1 + S_3 \otimes S_2 \otimes S_1 \\
+ S_0 \otimes S_1 \otimes S_2 + S_1 \otimes S_2 \otimes S_2 \\
+ S_2 \otimes S_1 \otimes S_3 + S_3 \otimes S_3 \otimes S_3. \tag{11}
\]

We present the following observation as a lower bound of Schmidt rank of \( U_8 \).

**Theorem 4** The Schmidt rank of tensor \( S_1 \otimes S_3 \otimes S_0 + S_2 \otimes S_0 \otimes S_1 + S_3 \otimes S_2 \otimes S_1 + S_1 \otimes S_2 \otimes S_2 + S_2 \otimes S_1 \otimes S_3 + S_3 \otimes S_3 \otimes S_3 \) is six. Furthermore \( \text{sr}(U_8) \geq 6 \).

**Proof** Let \( D = S_1 \otimes S_3 \otimes S_0 + S_2 \otimes S_0 \otimes S_1 + S_3 \otimes S_2 \otimes S_1 + S_1 \otimes S_2 \otimes S_2 + S_2 \otimes S_1 \otimes S_3 + S_3 \otimes S_3 \otimes S_3 \). Because \( U_8 \) can be projected onto \( D \) using a projector on the first system, we obtain that \( \text{sr}(D) \leq \text{sr}(U_8) \). So it suffices to prove \( \text{sr}(D) = 6 \) by contradiction. Suppose \( \text{sr}(D) \leq 5 \), namely \( D = \sum_{j=1}^{5} A_j \otimes B_j \otimes C_j \). Using the orthogonality of \( S_0, S_1, S_2, S_3 \) we obtain that \( S_2 \otimes S_0 + S_3 \otimes S_2, S_2 \otimes S_1 + S_3 \otimes S_3, S_1 \otimes S_2 \in \text{span}\{A_1 \otimes B_1, \ldots, A_5 \otimes B_5\} \). By setting \( A_1 \otimes B_1 = S_1 \otimes S_3 \) and \( A_2 \otimes B_2 = S_1 \otimes S_2 \), we obtain that \( S_0, S_1, S_2, S_3 \in \text{span}\{B_3, B_4, B_5\} \). It is a contradiction, so we have shown that \( \text{sr}(D) = 6 \).

Unfortunately we cannot determine \( \text{sr}(U_8) = 6 \) or 7 or 8, and we leave it as an open problem. In the next section, we shall show how to construct some three-qubit unitary operations of Schmidt rank from one to seven.
Fig. 1 The three-qubit Toffoli gate $T_3$ of Schmidt rank two can be realized using two CNOT gates and one CZ gate $\text{diag}(1, 1, 1, -1)$ in the middle. The CZ gate is locally equivalent to the CNOT gate via two Hadamard gates $H$. The local gate $X_A$ flips the qutrits $|0\rangle$ and $|2\rangle$.

### 3 Implementation of three-qubit unitary gates

We have shown in Theorem 3 the existence of three-qubit unitary gates of Schmidt rank one to seven. It is a natural question to ask how many CNOT gates $T := |0\rangle\langle 0| \otimes I_2 + |1\rangle\langle 1| \otimes \sigma_1$ are sufficient to implement them. In this section, we investigate the question. To save CNOT gates, we will construct three-qubit gates of various Schmidt rank different from those in Theorem 3. In particular, we show that the three-qubit Toffoli and Fredkin gate, respectively, have Schmidt rank two and four. We show in Theorem 5 that the combination of two CNOT gates and local unitary gates generate a three-qubit unitary gate of Schmidt rank one, two or four. So implementing gates of Schmidt rank three and larger than four requires at least three CNOT gates. In particular, we show in Theorem 6 that the combination of three CNOT gates can generate a three-qubit unitary gate of Schmidt rank seven, by using the isomorphism to the Strassen tensor from multiplicative complexity.

First, every Schmidt rank one unitary gate is a local unitary gate, and it does not require CNOT gate.

Second, the three-qubit gate $U_2 = I_A \otimes T_{BC}$ has Schmidt rank two and can be implemented using one CNOT gate. As it is trivial, we construct a nontrivial example. We point out that the known three-qubit Toffoli gate $T_3$ (i.e., the controlled CNOT gate) also has Schmidt rank two, because

$$T_3 = (I_2 \otimes I_2 \otimes H)(I_2 \otimes I_2 \otimes I_2 - 2|1\rangle\langle 1| \otimes |1\rangle\langle 1| \otimes |1\rangle\langle 1|)(I_2 \otimes I_2 \otimes H), \quad (12)$$

where $H = \begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{bmatrix}$ stands for the qubit Hadamard gate. It has been proven that the Toffoli gate can be implemented using three CNOT gates assisted with local gates [26,27], see Fig. 1.

Third, using the Toffoli gate and one more CNOT gate, we can construct a three-qubit gate $M_3$ of Schmidt rank three as follows.

$$M_3 = (T_{AB} \otimes H)T_3(I_2 \otimes I_2 \otimes H)$$

$$= (|0\rangle\langle 0| \otimes I_2 + |1\rangle\langle 1| \otimes \sigma_1) \otimes I_2 - 2|1\rangle\langle 1| \otimes |0\rangle\langle 1| \otimes |1\rangle\langle 1|. \quad (13)$$
The three-qubit gate $M_3$ of Schmidt rank three can be implemented using four CNOT gates, local Hadamard gates $H$ and local gate $X_A$ flipping the qutrit $|0\rangle$ and $|2\rangle$.

So we can realize $M_3$ using four CNOT gates assisted with local unitary gates in Fig. 2. We do not know whether four CNOT gates are also necessary for constructing a three-qubit unitary gate of Schmidt rank three. Nevertheless, it turns out that three CNOT gates are necessary. This is a corollary of the following observation.

**Theorem 5** The combination of two CNOT gates and local unitary gates generates a three-qubit unitary gate of Schmidt rank one, two or four.

**Proof** Up to the switch of systems, the combination of two CNOT gates and local unitary gates has the expression $M_1 = U_1(T_{AB} \otimes I_C)U(T_{AB} \otimes I_C)U_2$ or $M_2 = U_1((T_{AB} \otimes I_C)U(I_A \otimes T_{BC}))U_2$, with local three-qubit unitary gates $U_1$, $U$ and $U_2$.

One can verify that the first gate $M_1$ is indeed a two-qubit unitary gate, so it does not have Schmidt rank three. By choosing $U = I_8$, the gate $M_1$ becomes a local unitary gate.

Next we consider $M_2$. Suppose $U = V \otimes W \otimes X$ is a unitary matrix, where $V$, $W$, $X$ are $2 \times 2$ matrices. So $M_2$ also has the expression $M_2 = U_1(I_2 \otimes I_2 \otimes X)(T_{AB} \otimes I_C)(I_2 \otimes W \otimes I_2)(I_A \otimes T_{BC})(V \otimes I_2 \otimes I_2)U_2$. Because local unitary transformation does not change the Schmidt rank, we may assume that $U_1 = U_2 = I_8$ and $V = X = I_2$. We have

$$M_2 = (S_0 \otimes I_2 \otimes I_2 + S_3 \otimes \sigma_1 \otimes I_2)$$

$$= (I_2 \otimes W \otimes I_2)(I_2 \otimes S_0 \otimes I_2 + I_2 \otimes S_3 \otimes \sigma_1)$$

$$= S_0 \otimes W S_0 \otimes I_2 + S_0 \otimes W S_3 \otimes \sigma_1$$

$$+ S_3 \otimes \sigma_1 W S_0 \otimes I_2 + S_3 \otimes \sigma_1 W S_3 \otimes \sigma_1,$$

where $S_0, \ldots, S_3$ are the $2 \times 2$ matrices defined in (1). So $M_2$ has Schmidt rank at most four. It is clear that $S_0$ and $S_3$ are linearly independent in system $A$, $I_2$ and $\sigma_1$ are linearly independent in system $C$. We next consider the four matrices $W S_0$, $W S_3$, $\sigma_1 W S_0$ and $\sigma_1 W S_3$ in system $B$.

Assume that $k_1 W S_0 + k_2 \sigma_1 W S_0 + k_3 W S_3 + k_4 \sigma_1 W S_3 = 0$ for complex numbers $k_1$ to $k_4$ and set $W = \begin{bmatrix} m & n \\ l & p \end{bmatrix}$.

We obtain that

$$\begin{bmatrix} mk_1 + lk_2 & nk_3 + pk_4 \\ lk_1 + mk_2 & pk_3 + nk_4 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix},$$

(15)
and

$$mk_1 + lk_2 = 0, \quad (16)$$
$$lk_1 + mk_2 = 0, \quad (17)$$
$$nk_3 + pk_4 = 0, \quad (18)$$
$$pk_3 + nk_4 = 0. \quad (19)$$

There are two cases.

1. Suppose \( m^2 = l^2 \). Because \( U \) is a unitary matrix, we have \( n^2 = p^2 \). We obtain that \( WS_0 = \begin{bmatrix} m & 0 \\ l & 0 \end{bmatrix} \) and \( \sigma_1 WS_0 = \begin{bmatrix} l & 0 \\ m & 0 \end{bmatrix} \) are linearly dependent, \( WS_3 = \begin{bmatrix} 0 & n \\ 0 & p \end{bmatrix} \) and \( \sigma_1 WS_3 = \begin{bmatrix} 0 & p \\ 0 & n \end{bmatrix} \) are linearly dependent. Further,

$$M_2 = (S_0 + \frac{m}{l} S_3) \otimes WS_0 \otimes I_2$$
$$+ (S_0 + \frac{p}{n} S_3) \otimes WS_3 \otimes \sigma_1. \quad (20)$$

Note that \( WS_0 \) and \( WS_3 \) are linearly independent in system \( B \), so in this case \( M_2 \) has Schmidt rank two.

2. Suppose \( m^2 \neq l^2 \) and hence \( n^2 \neq p^2 \). Then from Eqs. (16) and (17) we obtain \( k_1 = k_2 = 0 \), from Eqs. (18) and (19), we obtain \( k_3 = k_4 = 0 \). It means that the four matrices in system \( B \) are linearly independent. Further, any three product matrices could not span the AB space of \( M_2 \). So in this case \( M_2 \) has Schmidt rank four.

We finish the proof.

Fourth, assume that \( W = I_2 \) in Eq. (14), we construct a three-qubit unitary gate \( M_4 = (T_{AB} \otimes I_C)(I_A \otimes T_{BC}) \). It is straightforward to prove that \( M_4 \) has Schmidt rank four. We describe it in Fig. 3. Note that two CNOT gates are the minimum cost of realizing every gate of Schmidt rank four. In contrast, we point out that the known three-qubit Fredkin gate \( F_3 \) (i.e., the controlled swap gate) also has Schmidt rank four, because

$$F_3 = (|0\rangle|0\rangle + \frac{1}{2}|1\rangle|1\rangle) \otimes I_2 \otimes I_2 + \frac{1}{2}|1\rangle|1\rangle \otimes \sigma_3 \otimes \sigma_3$$
$$+ |1\rangle|1\rangle \otimes |0\rangle|0\rangle + |1\rangle|1\rangle \otimes |1\rangle|0\rangle \otimes |0\rangle|1\rangle. \quad (21)$$

It has been proven that the Fredkin gate can be implemented using five CNOT gates assisted with local gates \([28]\), see Fig. 4.

Fifth, using the Fredkin gate and one more CNOT gate, we can construct a three-qubit gate \( M_5 \) of Schmidt rank five as follows.

$$M_5 = (T_{AB} \otimes I_2) F_3 = |0\rangle|0\rangle \otimes I_2 \otimes I_2$$
$$+ \frac{1}{2}|1\rangle|1\rangle \otimes \sigma_1 \otimes I_2 + \frac{1}{2}|1\rangle|1\rangle \otimes \sigma_1 \sigma_3 \otimes \sigma_3$$
The three-qubit gate $M_4$ of Schmidt rank four consists of two CNOT gates. This is minimum cost of realizing any three-qubit unitary gate of Schmidt rank four.

![Diagram](Fig. 3)

The three-qubit Fredkin gate $F_3$ of Schmidt rank four can be implemented using five CNOT gates and local gates $X_A$ flipping the qutrit $|0\rangle$ and $|2\rangle$.

![Diagram](Fig. 4)

The three-qubit gate $M_5$ of Schmidt rank five can be implemented using six CNOT gates and local gates $X_A$ flipping the qutrit $|0\rangle$ and $|2\rangle$.

![Diagram](Fig. 5)

We explain briefly why $sr(M_5) = 5$, as the proof is similar to that of constructing the gate in (2). First using (22), one can show that $5 \geq sr(U_5) \geq 4$. Next, if $sr(M_5) = 4$, then $M_5$ is the linear combination of four product matrices one of which has the form $S_0 \otimes I_2 \otimes I_2$. It can be excluded by comparing with (22). We have shown that $sr(M_5) = 5$. Using Fig. 4, we can implement $M_5$ using six CNOT gates assisted with local unitary gates in Fig. 5.

Sixth, using the gate $M_3$ in Fig. 2 and one more CNOT gate, we can construct a three-qubit gate $M_6$ of Schmidt rank six as follows.

$$M_6 = (T_{AC} \otimes (I_2)_B)(H \otimes I_2 \otimes I_2)M_3$$

$$= \frac{1}{\sqrt{2}} |0\rangle\langle 0| \otimes (I_2 \otimes I_2)$$

$$+ \frac{1}{\sqrt{2}} |0\rangle\langle 1| \otimes (\sigma_1 \otimes I_2 - 2|0\rangle\langle 1| \otimes |1\rangle\langle 1|)$$

$$+ \frac{1}{\sqrt{2}} |1\rangle\langle 0| \otimes I_2 \otimes \sigma_1$$

$$+ \frac{1}{\sqrt{2}} |1\rangle\langle 1| \otimes (2|0\rangle\langle 1| \otimes |0\rangle\langle 1| - \sigma_1 \otimes \sigma_1).$$

(23)
The three-qubit gate $M_6$ of Schmidt rank six can be implemented using five CNOT gates, Hadamard gate $H$ and qutrit gate $X_A$ flipping $|0\rangle$ and $|2\rangle$ where

$$H = \begin{bmatrix} \sqrt{2} & \sqrt{2} \\ \sqrt{2} & -\sqrt{2} \end{bmatrix}$$

is the Hadamard matrix. We explain briefly why $sr(M_6) = 6$, as the proof is similar to that of constructing the gate in (4). First Corollary 2 shows that $6 \geq sr(M_6) \geq 4$. Next if $sr(M_6) \leq 5$, then one can show that $\sigma_1 \otimes I_2 - 2|0\rangle\langle 1| \otimes |1\rangle\langle 1|$ and $2|0\rangle\langle 1| \otimes |0\rangle\langle 1| - \sigma_1 \otimes \sigma_1$ cannot be in the span of $I_2 \otimes I_2$, $I_2 \otimes I_2$ and any three product matrices. We have a contradiction and so $sr(M_6) = 6$. Using Fig. 2, we can implement $M_6$ using five CNOT gates assisted with local unitary gates in Fig. 6.

It remains to implement a three-qubit unitary gate of Schmidt rank seven using CNOT gates as few as possible. Fortunately this is the case by the following theorem.

**Theorem 6** The combination of three CNOT gates can generate a three-qubit unitary gate of Schmidt rank seven.

**Proof** Consider the expression $M_7 = (T_{AB} \otimes I_C)U_1(I_A \otimes T_{BC})U_2(T_{AC} \otimes (I_2)_B)$ where $U_1 = V_1 \otimes W_1 \otimes X_1$ and $U_2 = V_2 \otimes W_2 \otimes X_2$ are local three-qubit unitary gates.

Set $X_1 = I_2$, $W_2 = I_2$ and $V_1 V_2 = V$, we have

$$M_7 = (S_0 V S_0 \otimes W_1 S_0 + S_3 V S_0 \otimes \sigma_1 W_1 S_0) \otimes X_2$$

$$+ (S_0 V S_0 \otimes W_1 S_3 + S_3 V S_0 \otimes \sigma_1 W_1 S_3) \otimes \sigma_1 X_2$$

$$+ (S_0 V S_3 \otimes W_1 S_0 + S_3 V S_3 \otimes \sigma_1 W_1 S_0) \otimes X_2 \sigma_1$$

$$+ (S_0 V S_3 \otimes W_1 S_3 + S_3 V S_3 \otimes \sigma_1 W_1 S_3) \otimes \sigma_1 X_2 \sigma_1. \quad (24)$$

Next, assume $V_1 = I_2$, using the Hadamard gate $V_2 = H$. It is easy to show that the four matrices $S_0 V S_0$, $S_0 V S_3$, $S_3 V S_0$ and $S_3 V S_3$ in system $A$ are linearly independent. Assume $W_1 = I_2$, it is easy to show that the four matrices $W_1 S_0$, $W_1 S_3$, $\sigma_1 W_1 S_0$ and $\sigma_1 W_1 S_3$ in system $B$ are linearly independent. Next, assume $X_2 = H$ is also a Hadamard gate, and it implies the four matrices $X_2$, $\sigma_1 X_2$, $X_2 \sigma_1$ and $\sigma_1 X_2 \sigma_1$ in system $C$ are linearly independent.

Based on these conditions, we obtain that the three-qubit unitary gate

$$M_7 = (T_{AB} \otimes I_C)(I_A \otimes T_{BC})(T_{CA} \otimes (I_2)_B) \quad (25)$$

is isomorphic to the Strassen Tensor, and hence, it has Schmidt rank seven. We describe (25) in Fig. 7.

\[\square\]
Using Theorem 5, three CNOT gates are also necessary for implementing any three-qubit unitary gate of Schmidt rank seven. On the other hand, constructing the gates of Schmidt rank three to six in Figs. 2, 4, 5 and 6 costs more than three CNOT gates. It is an interesting problem to reduce the numbers or prove their necessity if possible.

4 Conclusions

We have constructed three-qubit unitary operations of Schmidt rank from one to seven, respectively. We have implemented them using CNOT gates and local unitary gates. It remains to determine whether the three-qubit unitary operations of Schmidt rank eight, nine and ten exist. It is also of interest to investigate their extension to multiqubit system for quantum circuits.

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