

A 12-CNOT Double Qubit Excitation Gate

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Abstract

Effective implementation of high-level quantum gates is essential for practical quantum computing. To the best of our knowledge, we present the first reported 12-CNOT decomposition of the double qubit excitation operator, improving upon state-of-the-art (SOTA) implementations with 13 CNOTs. Our new circuit has the lowest CNOT count (12), lowest CNOT depth (10), and lowest total circuit depth (16) among all the previous SOTA circuits. Further, we only added 2 extra one-qubit gates compared to the lowest one-qubit gate count (11) among the previous SOTA circuits.

1 Introduction

Effective implementation of important building blocks (such as high-level quantum gates) in quantum algorithms is essential for practical quantum computing. In this work, we look at one such high-level gate, the Double Qubit Excitation Operator, which implements the equation (1) (Eq. 20 of [21]):

$$U_{kl ij}(\theta) = \exp \left[-\frac{i\theta}{8} (X_i Y_j X_k X_l + Y_i X_j X_k X_l + Y_i Y_j Y_k X_l + Y_i Y_j X_k Y_l - X_i X_j Y_k X_l - X_i X_j X_k Y_l - Y_i X_j Y_k Y_l - X_i Y_j Y_k Y_l) \right]. \quad (1)$$

Using the computational-basis ordering $|q_i q_j q_k q_l\rangle$ in a 4-qubit system, the operator implements a continuous rotation between the two states $|0011\rangle$ and $|1100\rangle$, as shown in (2):

$$U(\theta) |x\rangle = \begin{cases} \cos \theta |0011\rangle + \sin \theta |1100\rangle, & |x\rangle = |0011\rangle, \\ \cos \theta |1100\rangle - \sin \theta |0011\rangle, & |x\rangle = |1100\rangle, \\ |x\rangle, & \text{otherwise.} \end{cases} \quad (2)$$

The double qubit excitation gate is used as a building block for several quantum algorithms, both near-term and fault-tolerant. In near-term algorithms, for example, it is used as a CNOT efficient alternative to the fermionic double excitation operator in variational ground-state ansätze such as unitary coupled cluster (UCCSD) [9, 10] in the Variational Quantum Eigensolver (VQE) and its adaptive variants such as QEB-ADAPT-VQE [20] and FAST-VQE [5]. In fault-tolerant algorithms, it is used in Trotterized Hamiltonian simulation and time evolution of the electronic-structure Hamiltonian [18]. Further, one can use the operator in state preparation, such as a UCC-type ansatz, for subsequent ground-state energy estimation in fault-tolerant algorithms like quantum phase estimation (QPE) [2].

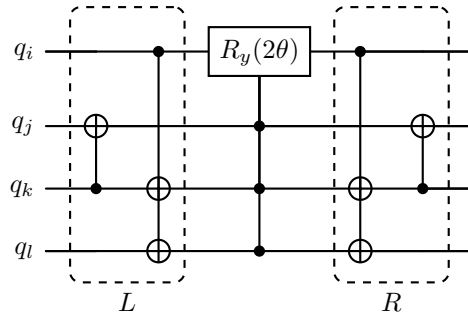


Figure 1 High-level double-excitation operator.

One can implement the double excitation gate simply using a triple controlled R_y rotation and some CNOT gates. Figure 1 shows such a high-level 4-qubit circuit with triple controlled $R_y(2\theta)$ rotation with q_i as the target qubit, sandwiched between L and R CNOT circuits. We refer to Yordanov *et al.* [21] for extended explanation on double qubit excitation operators, which is beyond the scope of this work. In this paper, we present, to the best of our knowledge, the first reported decomposition of the double-excitation operator with 12 CNOTs, improving on the previously reported SOTA implementations with 13 CNOTs.

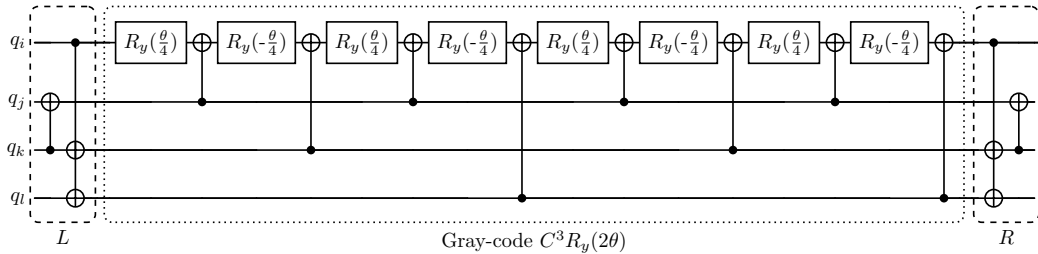
The structure of the rest of the paper is as follows. In Subsection 1.1, we will provide more details on the construction of the high-level circuit, including the role of L and R CNOT circuits. We also provide a simple 14-CNOT gate implementation using so-called Gray-code expansion [6, 15] of the $C^3R_y(2\theta)$ rotation. In Subsection 1.2, we will present the current SOTA implementations of the double excitation operator with 13-CNOTs. Finally in Section 2, we present a new 12-CNOT circuit for the double excitation operator. Our new circuit is better in 3 different metrics compared to existing SOTA circuits, i.e., in CNOT count (12), CNOT depth (10), and circuit depth (16).

1.1 A 14-CNOT baseline decomposition using Gray-code expansion

Recall that the double-excitation operator implements 8 Pauli strings, as shown in (1). One can naively implement the double-excitation operator of 48 CNOTs, implementing each of the 8 Pauli strings separately using 6 CNOT gates per string (see §4.7.3 and Fig. 4.19 of [8]). As discussed earlier, one can also implement the double-excitation operator using a single $C^3R_y(2\theta)$ rotation and some CNOT gates as shown in Figure 2. Intuitively, we want the controlled rotation to trigger only when the input state is either $|0011\rangle$ or $|1100\rangle$. Precisely, the L CNOT circuit performs this required transformation, as is defined in (3):

$$L|x\rangle = \begin{cases} |0111\rangle, & |x\rangle = |0011\rangle, \\ |1111\rangle, & |x\rangle = |1100\rangle, \\ |x'\rangle \text{ with } q_j q_k q_l \neq 111, & \text{otherwise,} \end{cases} \quad (3)$$

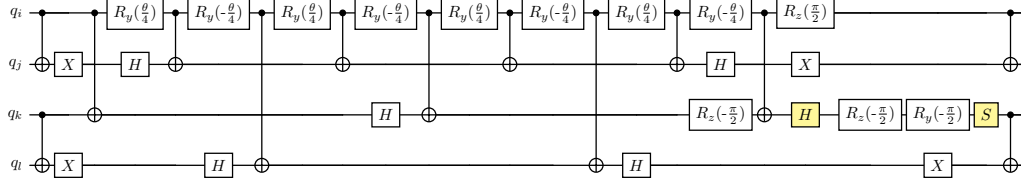
The R CNOT circuit, on the other hand, performs the inverse transformation of L , i.e., $LR = I$. Depending on the θ , controlled rotation $C^3R_y(2\theta)$ either flips the input basis states $|0011\rangle$ and $|1100\rangle$ or leaves them unchanged. Thus, all the input states excluding $|0011\rangle$ and $|1100\rangle$ stay untouched in the output, implementing our desired double-excitation operation. Decomposition of the triple-controlled R_y rotation is well studied, and multiple 8-CNOT constructions are known. Here, we use the Gray-code expansion of the $C^3R_y(2\theta)$ rotation [6, 15], with 8 CNOTs and 8 R_y rotations, resulting in a baseline 14-CNOT double-excitation gate as shown in Figure 2.



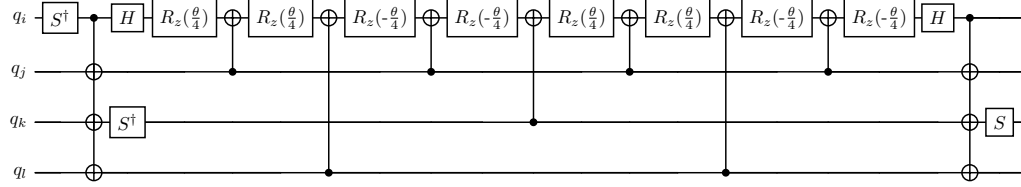
■ **Figure 2** A 14-CNOT decomposed double-excitation circuit with $C^3R_y(2\theta)$ Gray-code expansion.

1.2 Previous SOTA 13-CNOT double-excitation gate implementations

In the literature, several 13-CNOT decompositions of the double-excitation operator have been proposed. The usual approach is to find rewrite rules to absorb some of the CNOTs in the L and R circuits into the various decompositions of the $C^3R_y(2\theta)$ rotation, resulting in 13-CNOT circuits. Later in Table 1, we refer to some well-known examples of these 13-CNOT circuits of the double-excitation operator, and their metrics. In this Subsection, we present two of the best 13-CNOT circuits from the literature. The 13-CNOT circuit by Yordanov



■ **Figure 3** A 13-CNOT double-excitation gate by Yordanov et al. [21, 20] with lowest CNOT depth (11) cf. Table 1. The two highlighted gates on q_k are added to correct the original circuit.

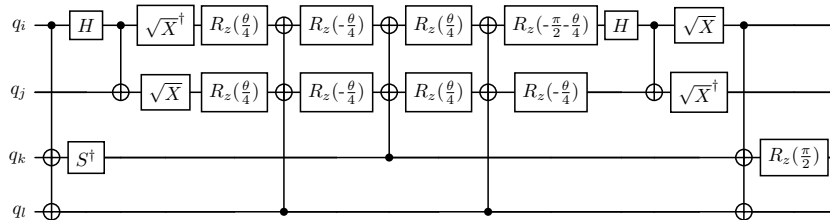


■ **Figure 4** Nam [7] double-excitation circuit with 13 CNOTs. Among the 13-CNOT reference circuits it has the lowest one-qubit gate count (11). Cf. Table 1.

et al. [21, 20] as shown in Figure 3 has the lowest 11 CNOT depth but at the cost of 16 one-qubit gates. Figure 4 on the other hand shows a 13-CNOT circuit by Nam [7] with the lowest one-qubit gate count (11) but at the cost of 13 CNOT depth. Another 13-CNOT circuit by Wang [18] is reported in the Table 1 with 15 one-qubit gates and 13 CNOT depth.

2 A 12-CNOT decomposition of the double-excitation operator

Although several 13-CNOT decompositions of the double-excitation operator have been proposed in the literature, our literature search found no previously reported implementation with fewer than 13 CNOTs. In this section, we present the first 12-CNOT decomposition of the double-excitation operator, as shown in Figure 5. We have used various circuit synthesis



■ **Figure 5** Our best double-excitation circuit: 12 CNOTs (same-control CNOTs drawn compactly as fan-outs, but expanded when computing depth), CX-depth 10, 13 one-qubit gates. Cf. Table 1.

■ **Table 1** CNOT count, CNOT depth, single-qubit gate count, and total circuit depth for double-excitation circuit implementations. Single-qubit gates are counted as universal one-qubit (u3) gates, i.e., each maximal run of consecutive single-qubit gates on a qubit is merged into one u3 gate.

Circuit	CX count	CX depth	1q gates	Depth
Naive Pauli decomposition [8]	48	48	38	64
Baseline: with Gray-code (Fig. 2) [6, 15]	14	14	8	22
PennyLane 2021 [1, 19]	14	12	14	20
Wang 2021 [18]	13	13	15	22
Nam 2020 [7]	13	13	11	22
Yordanov 2020 [21, 20]	13	11	16	20
This work (Fig. 5)	12	10	13	16

and optimization tools such as Q-Synth [11], Qiskit Transpiler [3], Tket [16] to explore different decompositions of the double-excitation operator. Various synthesis techniques such as Clifford Synthesis [13, 14], CNOT+Rz Synthesis [12, 4], KAK decomposition [17] etc. have been useful to extensively explore different decompositions (mainly for excluding dead ends). Table 1 compares our new 12-CNOT circuit with the previous SOTA 13-CNOT circuits, in 4 different metrics. Our new circuit has the lowest CNOT count (12), lowest CNOT depth (10), and lowest total circuit depth (16) among all the previous SOTA circuits.

3 Conclusion

In this work, we presented, to the best of our knowledge, the first reported 12-CNOT decomposition of the double qubit excitation operator. We compared our new circuit with the previous SOTA 13-CNOT circuits in 4 different metrics. Our new circuit has the lowest CNOT count (12), lowest CNOT depth (10), and lowest total circuit depth (16) among all the previous SOTA circuits. Further, we only added 2 extra one-qubit gates compared to the lowest one-qubit gate count (11) among the previous SOTA circuits.

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