Decomposition of Toffoli gates for MCX optimization

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Project description

The multi-controlled Toffoli (MCX) gate is essential to many quantum operations including the Glover operator, logical AND, various state preparation algorithms, and arithmetic comparators. The decomposition of complex controlled operations (like CCX, and CCCX) can be implemented using a circuit built from elementary operations. However, it is very complicated to contract MCX in minimum depth which is helpful in practical large-scale designs.

In this project, we report the standard decomposition of CCX & CCCX gates using the unitary U & CX gate and $R_y(\theta)$ based decomposition using qiskit library. We proposed reduced Toffoli gates without preserving control qubits and to find the best way to construct n-controlled MCX gate automatically, we used classical optimizer. We also discussed the spectral decomposition of MCX using a qiskit pulse.

Keywords: Multi-controlled Toffoli, CCX, CCCX decomposition, Spectral decomposition

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1. Standard decomposition of CCX & CCCX

A Toffoli gate, or CCX gate can be decomposed into 6 CXs and 9 Unitary gates. However, its standard decomposition into CX and single unitary gates in the Qiskit library is not itself symmetric. Among these gates, 2 CX and 3 unitary gates are used for preserving the control qubits which do not involve the target qubit.

If we have a look at the decomposition of the Toffoli gate:
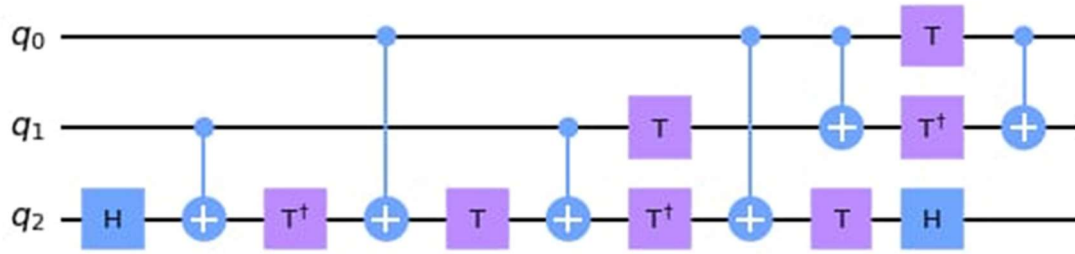
In practical large-scale design, we construct multiply controlled gates using ancillary qubits, such as the one described in Nielsen & Chuang, fig. 4.10:
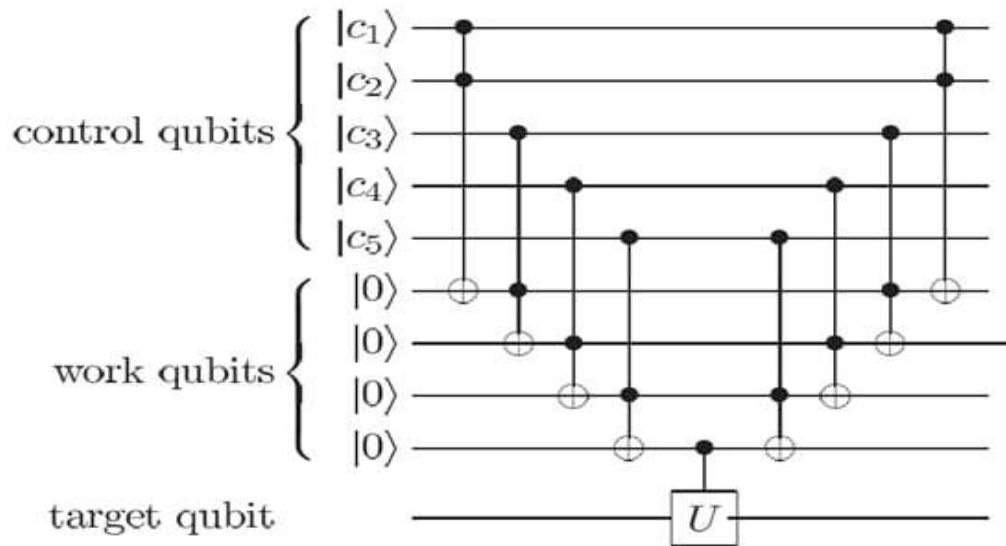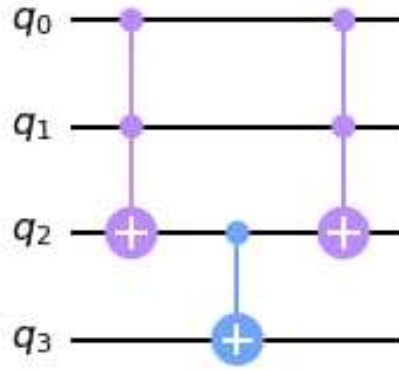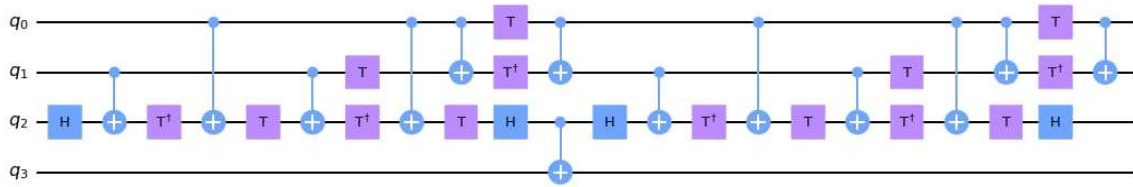

Figure 4.10. Network implementing the $C^n(U)$ operation, for the case $n = 5$.
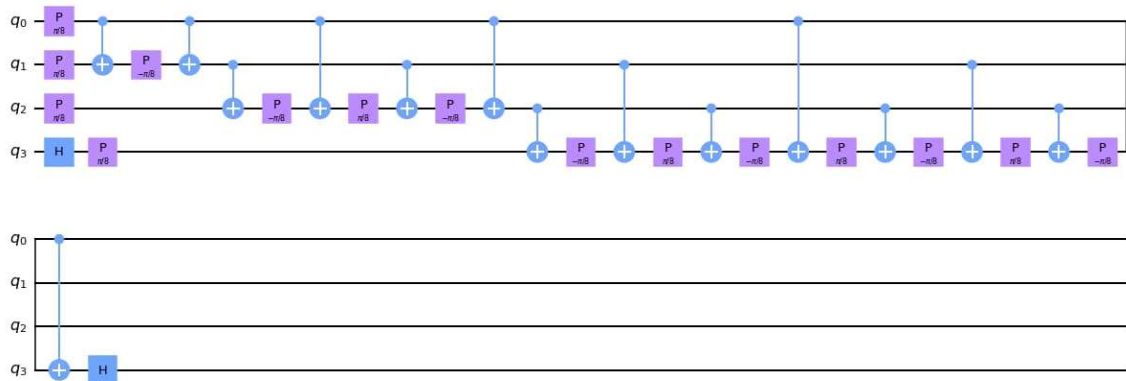
A Toffoli gate can be represented by the following circuit using an ancillary qubit:

In current transpiler, the circuit will decompose in 12 CXs and 14 T-gates and also requires the underlying layout to have a connection between qubits 1 and 2.
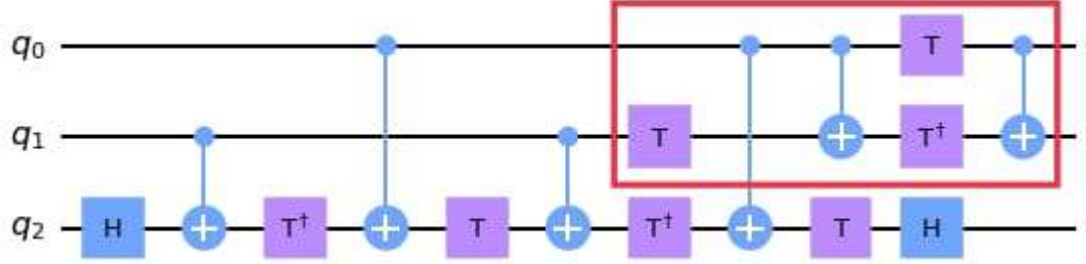

Similarly, current decomposition of a CCCX (an MCX gate with 3 controls) it looks like:
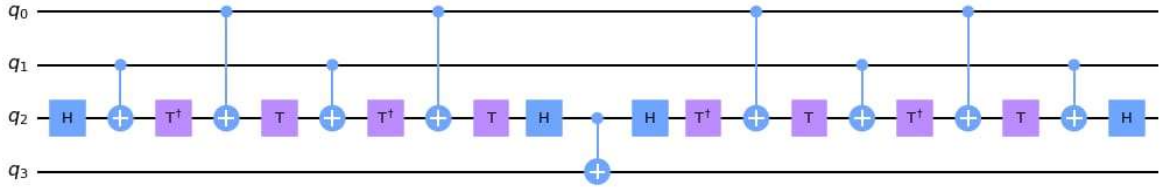
2. Reduced Toffoli gate

Without preserving control qubits, the reduced Toffoli gate can be decomposed in 4 CX and 6 Unitary gates.

And the same above circuit can be decomposed in 8 CXs and 8 T-gates, the standard transpiler will cancel the 5 operations using the reduced Toffoli gate and produce the following result:

To construct a large network of multiply controlled gates, our reduced Toffoli gate provides significant improvement in complexity and depth.
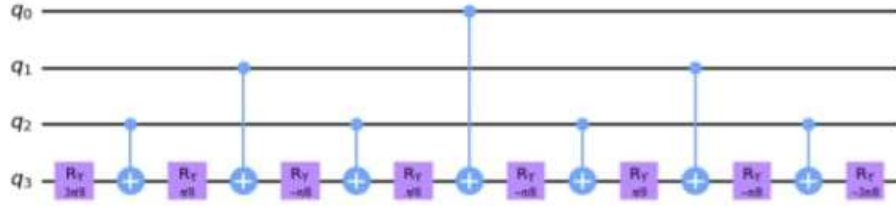
3. $R_y(\theta)$-based Toffoli gate

Another way to construct a Toffoli gate is down below. This gate only uses 3 CXs and 4 Unitary gates but requires the destination qubit to be clean
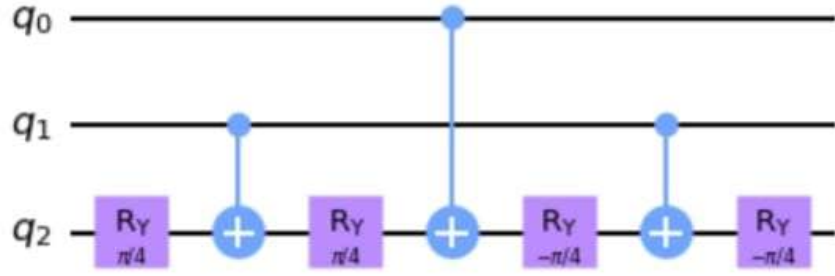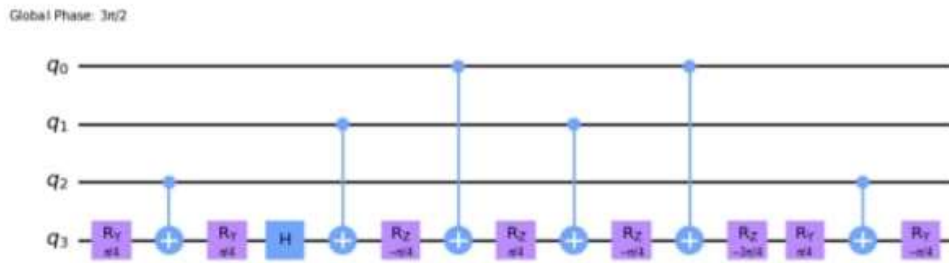
4. R$_y$(θ)-based CCCX gate

R$_y$(ϑ)-based CCCX gates decomposition is described below:

It can be executed with fewer elementary gates using a reduced Toffoli gate by replacing the 2nd CX gate.

5. General n-controlled MCX gate

Any n-controlled MCX can be decomposed in reduced CCX and CCCX gates. But to find the best solution with minimum depth, we need to add them in an appropriate order, which can be done by a classical optimizer. When calculating the circuit depth, we can arrange the order of input qubits so that the depth will be minimized.

6. Discussion

In the current transpiler, the decomposition of MCX is not optimal, which increases complexity and circuit depth. We provided better decomposition with reduced Toffoli gate and an optimal solution for this problem. This problem can be analysed by Qiskit Pulse, which is a low-level pulse-programming paradigm implemented as a module within Qiskit Terra and gives the user precise control over working at the real quantum hardware level, the ability to calibrate and execute pulse, and read-out level instructions. We can use the Qiskit Pulse model to calibrate and create MCX gates with high fidelity. We could start by calibrating the qubit frequency of qubit 0 at IBMQ Armonk backend, accurately by the frequency sweep method. We can perform calibration of Toffoli Gate by defining and varying the pulse parameters, in different cloud-based IBM backends to higher fidelity.

7. Reference:

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[4] Building pulse schedules — qiskit 0.37.0 documentation.