

Pierre-Antoine Graham

## HOMEWORK 2

Eduardo Martín-Martínez, Bindiya Arora  
*Quantum Information*

Perimeter Institute for Theoretical Physics  
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# 1 Back to basics: quantum circuits

In what follows, we evaluate the matrix expressions representing a quantum circuit unitary acting on a sequence of qubit input. We work in the computational basis  $\{|0\rangle, |1\rangle\}$  and use the notation  $X, Y, Z$  for the Pauli gates in this basis.

- (a) First we consider the conjugation of a CNOT by two CNOT with control and target qubit reversed:

$$\begin{array}{c} 1 \\ 2 \end{array} \begin{array}{c} \oplus \\ \bullet \\ \oplus \\ \bullet \end{array} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

which exchanges the qubits ( $|00\rangle \rightarrow |00\rangle, |01\rangle \rightarrow |10\rangle, |10\rangle \rightarrow |01\rangle, |11\rangle \rightarrow |11\rangle$ ) and constitutes a SWAP gate. The matrix expression for the reversed CNOT was obtained by writing its action on the computational basis which reads  $|00\rangle \rightarrow |00\rangle, |01\rangle \rightarrow |11\rangle, |10\rangle \rightarrow |10\rangle, |11\rangle \rightarrow |01\rangle$ .

- (b) Then we calculate the matrix expression of the entanglement-generating circuit

$$\begin{array}{c} 1 \\ 2 \end{array} \begin{array}{c} \oplus \\ \bullet \\ \oplus \\ \bullet \end{array} = (1_1 \otimes |0\rangle \langle 0|_2 + X_1 \otimes |1\rangle \langle 1|_2) R_{\pi/4,2} \left( 1_1 \otimes \frac{1}{\sqrt{2}} (X_2 + Z_2) \right) \\ = (1_1 \otimes |0\rangle \langle 0|_2 + X_1 \otimes e^{i\pi/4} |1\rangle \langle 1|_2) \left( 1_1 \otimes \frac{1}{\sqrt{2}} (X_2 + Z_2) \right) \\ = \frac{1}{\sqrt{2}} (1_1 \otimes |0\rangle_2 \langle 0|_2 + |1\rangle_2 \langle 1|_2 + X_1 \otimes e^{i\pi/4} |1\rangle_2 \langle 0|_2 - |1\rangle_2 \langle 1|_2) = \frac{1}{\sqrt{2}} \left( \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ e^{i\pi/4} & -e^{i\pi/4} \end{pmatrix} \right) \\ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & e^{i\pi/4} & -e^{i\pi/4} \\ 0 & 0 & 0 & 0 \\ e^{i\pi/4} & -e^{i\pi/4} & 0 & 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & e^{i\pi/4} & -e^{i\pi/4} \\ 0 & 0 & 1 & 1 \\ e^{i\pi/4} & -e^{i\pi/4} & 0 & 0 \end{pmatrix}.$$

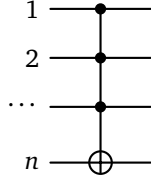
If we set the phases to 1, we recover the Bell state mapping  $|00\rangle \rightarrow (|00\rangle + |11\rangle)/\sqrt{2}, |01\rangle \rightarrow (|00\rangle - |11\rangle)/\sqrt{2}, |10\rangle \rightarrow (|01\rangle + |10\rangle)/\sqrt{2}$  and  $|11\rangle \rightarrow (-|01\rangle + |10\rangle)/\sqrt{2}$ .

- (c) Finally, we calculate the matrix expression associated with a three-qubit circuit as follows:

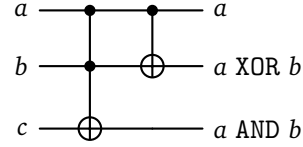
$$\begin{array}{c} 1 \\ 2 \\ 3 \end{array} \begin{array}{c} \oplus \\ \bullet \\ \oplus \\ \bullet \end{array} = \text{TOFFOLI } R_{\pi/4,3} H_2 (|0\rangle \langle 0|_1 \otimes 1_2 + |1\rangle \langle 1|_1 \otimes X_2) H_1 \\ = \text{TOFFOLI } R_{\pi/4,3} \frac{1}{\sqrt{2}} (|0\rangle_1 \langle 0|_1 + |1\rangle_1 \langle 1|_1) \otimes H_2 + |1\rangle_1 \langle 0|_1 \otimes H_2 X_2 \\ = \text{TOFFOLI } R_{\pi/4,3} \frac{1}{2} \left( \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & -1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \right) \\ = \text{TOFFOLI } R_{\pi/4,3} \frac{1}{2} \left( \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & -1 & -1 \\ -1 & 1 & 1 & -1 \end{pmatrix} \right) \\ = \text{TOFFOLI } R_{\pi/4,3} \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & 1 & 1 & -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1_3 & 0 & 0 & 0 \\ 0 & 1_3 & 0 & 0 \\ 0 & 0 & 1_3 & 0 \\ 0 & 0 & 0 & X_3 \end{pmatrix} R_{\pi/4,3} \begin{pmatrix} 1_3 & 1_3 & 1_3 & 1_3 \\ 1_3 & -1_3 & 1_3 & -1_3 \\ 1_3 & 1_3 & -1_3 & -1_3 \\ -1_3 & 1_3 & 1_3 & -1_3 \end{pmatrix}.$$

## 2 Quantum Adder

- (a) The TOFFOLI gate can be generalized to  $n$  qubits by increasing the number of control qubit to  $n - 1$  conditioning a NOT operation on qubit  $n$ . The circuit corresponding to this generalization is presented in Fig. 1 (a).



(a)  $n$ -qubit generalisation of the TOFFOLI gate.



(b) Circuit for the addition of two single-bit numbers  $a$  and  $b$ .

Figure 1: Circuits for 2 (a) and 2 (b).

- (b) Given two single-digit binary numbers  $a$  and  $b$ , we can calculate  $a + b$  with a quantum circuit by encoding them in input numbers in qubit states  $|a\rangle$  and  $|b\rangle$  where the digit forms the 0,1 label of a computation basis element. In other words, the classical bit adder algorithm can be implemented with a quantum circuit. This algorithm requires qubits for inputs  $a$  and  $b$  and a qubit initialized to  $|0\rangle$  that will eventually be updated to store the carry-on of  $a + b$  (if we add  $1 + 1$  we get 10 which is represented here by having 1 stored in the carry on qubit, and 0 stored in the output state for the  $b$  qubit Hilbert space. The state of  $a$  is unchanged to allow for the reversibility of calculation and its implementation as a sequence of unitary operations). The Quantum circuit implementing the single is presented in Fig. 1 (b). On one hand, the TOFFOLI gate flips the carry-on  $c$  to 1 iff both  $a$  and  $b$  are initialized to 1. On the other hand, the CNOT gate replaces the value of  $b$  by  $a \text{ XOR } b$  storing the first digit of the addition output in  $b$ .
- (c) If we consider adding 4 binary numbers  $a, b, c, d$  together, we need an additional carry-on qubit to represent the result since  $1 + 1 + 1 + 1 = 100$  requires 3 qubits to describe its digits. In this case, we name the carry-on  $c_1$  and  $c_2$ . The circuit performing the addition of 4 single-bit numbers together is presented in Fig. 2 The first two layers of this circuit add  $a$  and  $b$  in the way explained in (b). At the

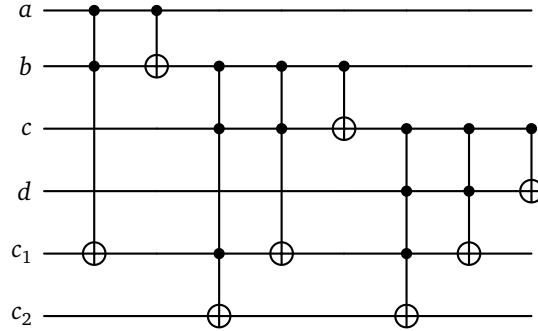


Figure 2: Circuit for the addition of four single bit numbers  $a, b, c, d$ . The output is stored in qubit  $d$  (first digit),  $c_1, c_2$  (last digit)

second layer, the CNOT operation shifts the last digit output to the  $b$  qubit. The next group of operations uses the value stored in  $b, c, c_1$  to add the updated  $b$  and  $c$  while taking the  $c_1$  carry-on into account. The first gate of the third layer flips  $c_2$  iff  $b, c, c_1$  are all one (in our case this does not happen because  $c_1 = 0$  implies  $b = 0$ ). The fourth and fifth layers are copies of the operations described in (b) acting on  $b, c, c_1$ . At the fifth layer, the CNOT operation shifts the last digit output to the  $c$  qubit. At layer six, a generalized TOFFOLI is applied to possibly flip the  $c_2$  carry-on if  $c, d, c_1$  are all 1 (which is a real possibility in this case). The seventh layer updated the value of the  $c_1$  carry on from the values of  $c, d$  (if it was 1 and gets a 1 contribution from  $c, d$ , it is flipped to 0). The required carry-on to  $c_2$  associated with this flip was already done by the sixth layer). At the last layer, the CNOT operation shifts the last digit output to the  $d$  qubit. The final output of the addition is stored in qubits  $d, c_1, c_2$ .

## 3 Grover's algorithm on IBM composer

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- (1) The Grover algorithm is implemented in three parts. The first part is a layer of Hadamard gates preparing the qubits initialized to 0 in a uniform superposition of all binary strings in which we need to search. The second part consists in applying NOT gates to go to a basis where the target string is mapped to  $1 \cdots 1$ . Then, in that basis, a generalized CZ operation is applied to the last qubit and controlled by all other qubits. This operation plays the role of the oracle applying a  $-1$  factor to the desired state only. To go back to the initial computational basis, we then apply NOT gates to undo the previous basis transformation. In practice, a generalized CZ gate can be constructed by conjugating a generalized CNOT by two Hadamard gates on the target qubit space. Since  $H^2 = 1$  (if controls do not activate, we apply 1) and  $HXH = Z$  (if controls activate, we apply  $Z$ ), this indeed realizes a generalized CZ. The third step consists of applying a reflection with respect to state  $|s\rangle$  which is a uniform superposition of all states. To perform that reflection, we first move to a basis where this state is moved to  $1 \cdots 1$ . This is done by first applying Hadamard gates to all qubits (mapping  $|s\rangle$  to the state with binary string  $0 \cdots 0$ ) and then applying NOT to all of them (mapping  $0 \cdots 0$  to  $1 \cdots 1$ ). In this basis, a generalized CZ (with a target on the last qubit and controlled by all other qubits) is applied to add a  $-1$  phase only to the  $1 \cdots 1$  (In the geometric interpretation of Grover's algorithm, the reflection applies a  $-1$  phase to all components except the  $|s\rangle$  component. What is done here differs from this operation by a global  $-1$  phase and produces the same results at the measurement step). We finally return to the computational basis by applying a layer of NOT gates followed by a layer of Hadamard gates. See the example circuits linked in the `Circuits.txt` file.

## 4 Acknowledgement

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Thanks to Jonathan for a discussion about the quantum adder.