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Quantum Computing Project: Report

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1 Introduction

1.1 Aims

1.2 Background

The history of computers reaches back to the middle of the 19th century when a design for an Analytical Engine was proposed by Charles Babbage who is considered to be one of the early pioneers of computation. However, for almost 100 years this branch stayed an interesting but rather conceptional one until the invention of the transistor in 1925. The first working computers were built in the 1940s and up to today computers work principally the same way.

Quantum computation on the other hand is a quite recent research field which emerged from the physics of quantum mechanics (1920s). In 1982 Richard Feynman theorised that there seemed to be essential difficulties in simulating quantum mechanical system on classical computers and suggested that a quantum computer would solve these issues.[4]

Remarkable theoretical breakthroughs in the 1990s followed, when Peter **Shor** demonstrated that essential problems – like factorising integers – could be solved far more efficiently on quantum computers than on conventional, classical computers. Besides Shor's algorithm Lov **Grover** proposed another algorithm in 1995 (only one year later) showing that the problem of conducting a search through some unstructured search space is as well more efficient on quantum computers.

The practical challenges for building a quantum computer are high and therefore the realisation of real quantum computers is still in it's infancy. However, in 2001 the first real quantum computer was able to factorise 15 into its prime numbers (3 and 5) by using a 7-qubit system.[6] Since then experimental progress is booming but the state-of-the-art is still a fair way off from practical (and even less daily-life) usage.

2 Theory

In this chapter we introduce the basic concepts of quantum computation, starting off with definitions of **qubits**, **quantum registers** and the presentation of several **quantum gates**. Afterwards we will talk about two **quantum algorithms** that we implemented in our virtual quantum computer. The last chapter will briefly talk about the challenges of **building a real quantum computer**.

2.1 Qubits

2.1.1 Generalised bits

A qubit (from *qu*antum *bit*) is the smallest unit in a quantum computer and therefore the quantum mechanical **generalisation of a classical bit**, as it is used in computers nowadays. A classical bit has one and only one of the two possible states

$$|0\rangle \quad \text{or} \quad |1\rangle \tag{1}$$

at the same time, whereas a qubit is able to be in a state $|\Psi\rangle$ which is a superposition of these two classical states:

$$|\Psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,, \quad \text{where } |\alpha|^2 + |\beta|^2 = 1 \tag{2}$$

One can depict the states via matrices with basis $(|0\rangle\,, |1\rangle)$:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad |\Psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{3}$$

2.1.2 Measurement

The superposition of states leads to a new understanding of measurement. There are two things to consider:

1. **Probabilities** P
   Given a classical state ($|\Psi\rangle$ either $|0\rangle$ or $|1\rangle$) the result of a measurement is certain (and trivial). That's no longer true for the quantum state: Given the state $|\Psi\rangle$ in Eq. 2, it is solely possible to calculate the **probabilities** P_Ψ of the outcome:

$$P_\Psi(0) = |\langle 0|\Psi\rangle|^2 = \left|\alpha \underbrace{\langle 0|0\rangle}_{=1} + \beta \underbrace{\langle 0|1\rangle}_{=0}\right|^2 = |\alpha|^2 \tag{4}$$

$$P_\Psi(1) = |\langle 1|\Psi\rangle|^2 = \left|\alpha \underbrace{\langle 1|0\rangle}_{=0} + \beta \underbrace{\langle 1|1\rangle}_{=1}\right|^2 = |\beta|^2 \tag{5}$$

2. **Collapse of** $|\Psi\rangle$
   In classical measurements it is fair to say that the measurement itself has no (noticeable) influence on the result. This is no longer true in quantum mechanics: The wave function $|\Psi\rangle_i$ **collapses after a measurement** to a projection onto the measured eigenstate and therefore becomes a different state $|\Psi\rangle_f$:

$$|\Psi\rangle_i = \alpha\,|0\rangle + \beta\,|1\rangle \quad \xrightarrow{\text{Measurement: Value } m} \quad |\Psi\rangle_f = \begin{cases} |0\rangle\,, \text{ if } m = 0 \\ |1\rangle\,, \text{ if } m = 1 \end{cases} \tag{6}$$

2.2 Quantum register

A quantum register of size n is a **collection of** n **qubits**. Therefore we get $N \equiv 2^n$ basic states:

$$|b_{n-1}\rangle \otimes |b_{n-2}\rangle \otimes ... \otimes |b_1\rangle \otimes |b_0\rangle \tag{7}$$

where $b_i \in \{0, 1\}$. One can interpret this chain of zeros and ones as binary code, able to store numbers in the range of $[0, 1, ..., N-1]$. For example for a 3-qubit system we get:

$$\begin{aligned} |0\rangle \otimes |0\rangle \otimes |0\rangle &\equiv |000\rangle \equiv |0\rangle & \qquad |1\rangle \otimes |0\rangle \otimes |0\rangle &\equiv |100\rangle \equiv |4\rangle \\ |0\rangle \otimes |0\rangle \otimes |1\rangle &\equiv |001\rangle \equiv |1\rangle & \qquad |1\rangle \otimes |0\rangle \otimes |1\rangle &\equiv |101\rangle \equiv |5\rangle \\ |0\rangle \otimes |1\rangle \otimes |0\rangle &\equiv |010\rangle \equiv |2\rangle & \qquad |1\rangle \otimes |1\rangle \otimes |0\rangle &\equiv |110\rangle \equiv |6\rangle \\ |0\rangle \otimes |1\rangle \otimes |1\rangle &\equiv |011\rangle \equiv |3\rangle & \qquad |1\rangle \otimes |1\rangle \otimes |1\rangle &\equiv |111\rangle \equiv |7\rangle \end{aligned}$$

We call this collection the **computational basis** of our register.

However, in contrast to a classical system, a quantum register is able to be in a **state of superposition** which turns out to be the fundamental advantage for quantum computation. If for example the second qubit is set to a superposition $|\Psi_{b_1}\rangle = \frac{1}{\sqrt{2}} \binom{+1}{-1}$ the total state of the register will be:

$$\begin{aligned} \left|\Psi^{\text{tot}}\right\rangle &= |\Psi_{b_2}\rangle \otimes |\Psi_{b_1}\rangle \otimes |\Psi_{b_0}\rangle & (8) \\ &= |0\rangle \otimes \left[\tfrac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)\right] \otimes |1\rangle & (9) \\ &= \tfrac{1}{\sqrt{2}}\left[|001\rangle - |011\rangle\right] & (10) \\ &\equiv \tfrac{1}{\sqrt{2}}\left[|1\rangle - |3\rangle\right] & (11) \end{aligned}$$

Eq. 11 is always reducible to a (tensor) product of three single states, as Eq. 8 suggests. This is not always the case. Consider the 2-qubit system where

$$\left|\Psi^{\text{ent}}\right\rangle = \frac{1}{\sqrt{2}}\left[|00\rangle + |11\rangle\right]. \tag{12}$$

There is no way to separate this wave function into a (tensor) product of two states $\{|\Psi_{b_1}\rangle, |\Psi_{b_0}\rangle\}$. Thus, the state $|\Psi^{\text{ent}}\rangle$ is called **entangled**.

2.3 Quantum gates

After defining the quantum register, we now want to process it through a number of so-called quantum gates. These are (mathematically spoken) **unitary operations** applied to our register in order to change its total state $|\Psi^{\text{tot}}\rangle$. Since we work in the Hilbert space, all our operations are **linear**, therefore we can represent any gate working on a n-qubit register by a $N \times N$ matrix.

In the following subsections we will first introduce the most important gates used in our project, and then speak about generalisations of these gates for bigger registers.

2.3.1 Not gate

The first example for a simple 1-qubit gate is the Not-gate. It simply maps the state $|0\rangle \to |1\rangle$ and vice versa and is therefore equivalent to a logic NOT. The representing matrix in the computational basis $\{|0\rangle, |1\rangle\}$ is:

$$G^{\text{not}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{13}$$

$$G^{\text{not}}|0\rangle = |1\rangle \tag{14}$$

$$G^{\text{not}}|1\rangle = |0\rangle \tag{15}$$

However, this gate exists in exactly the same form for classical computation.

2.3.2 Hadamard gate

A common gate in quantum computation is the Hadamard gate. It performs the Hadamard transformation on a single qubit system in the following way:

$$G^{\text{H}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{16}$$

$$G^{\text{H}}|0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \tag{17}$$

$$G^{\text{H}}|1\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}} \tag{18}$$

The Hadamard gate is a 'real' quantum gate since it is able to set the state to a superposition of basic states.

For a n-qubit system it is necessary to define on which qubit a gate is acting. In the following we will use the subscript to depict this: The gate G_k is acting on the k-th qubit.

Note that a combination of Hadamard gates acting on every single qubit in a n-qubit register

with initial state $|\Psi\rangle = |00...0\rangle$ will lead to an **uniform superposition** of all basic states:

$$\left(\prod_{k=0}^{n-1} G_k^{\mathrm{H}}\right)|\Psi\rangle = G_{n-1}^{\mathrm{H}} \underbrace{|b_{n-1}\rangle}_{=|0\rangle} \otimes ... \otimes G_0^{\mathrm{H}} \underbrace{|b_0\rangle}_{=|0\rangle} \tag{19}$$

$$= \tfrac{|0\rangle+|1\rangle}{\sqrt{2}} \otimes ... \otimes \tfrac{|0\rangle+|1\rangle}{\sqrt{2}} \tag{20}$$

$$= 2^{-\frac{n}{2}} \sum_{k=0}^{N-1} |k\rangle \tag{21}$$

2.3.3 Phase gate

The Hadamard gate already uses special properties of quantum computation, but all operations are part of the real subspace of the Hilbert space. In general the gates and quantum register can operate on a complex vector space. The phase gate is such a gate which is defined for a single qubit system as:

$$G^{\phi} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} \tag{22}$$

$$G^{\phi}|0\rangle = |0\rangle \tag{23}$$

$$G^{\phi}|1\rangle = e^{i\phi}|1\rangle \tag{24}$$

2.3.4 Extension to bigger registers

As roughly mentioned before, any single qubit gate can by applied to the k-th qubit of a n-qubit register. Consider for example an arbitrary gate G_1 in a 2-qubit system. The resulting matrix G_{tot} is:

$$G_{\mathrm{tot}} = G_1 \otimes \underbrace{G_0}_{=\mathbb{I}_2} \tag{25}$$

$$= \begin{pmatrix} g_{00} & g_{01} \\ g_{10} & g_{11} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{26}$$

$$= \begin{pmatrix} g_{00}\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) & g_{01}\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) \\ g_{10}\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) & g_{11}\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) \end{pmatrix} \tag{27}$$

$$= \begin{pmatrix} g_{00} & 0 & g_{01} & 0 \\ 0 & g_{00} & 0 & g_{01} \\ g_{10} & 0 & g_{11} & 0 \\ 0 & g_{10} & 0 & g_{11} \end{pmatrix} \tag{28}$$

The general expression for n-qubit systems is analogous:

$$G_{\mathrm{tot}} = G_{n-1} \otimes ... \otimes G_k \otimes ... \otimes G_0 \tag{29}$$

$$= \mathbb{I}_2 \otimes ... \otimes \left(\begin{smallmatrix} g_{00} & g_{01} \\ g_{10} & g_{11} \end{smallmatrix}\right) \otimes ... \otimes \mathbb{I}_2 \tag{30}$$

2.3.5 Gate representations

The resulting matrix G_{tot} is in general a $N \times N$-matrix with two and only two non-zero entries in every row and column. That means that only $2 \cdot 2^n$ of 2^{n^2} entries are non-zero. The ratio is 2^{1-n} which rapidly goes towards zero for big n. Thus, most entries of the gate matrices will be zero.

This leads to the consideration of the following three possible representations:

1. **Dense matrix representation**
   A dense matrix representation is the standard representation, storing every single entry of a matrix. This leads to two major disadvantages in our special case:

   (a) *Memory*
   A classical computer reserves a certain amount of memory for every entry of a conventional matrix, no matter if the value is zero or non-zero. Therefore using dense matrices for big quantum registers might cause a serious lack of working memory.

   (b) *Calculation*
   We get a lot of trivial (and unnecessary) calculations using the standard matrix multiplication rule.

   The quantum register, however, has mostly non-zero entries for most of the steps of the usual algorithms.

2. **Sparse matrix representation**
   A sparse matrix representation only stores non-zero elements of a matrix in a list. Therefore every non-zero element requires a positioning index and the number itself to store.

3. **Functional representation**
   Since there are only two non-zero elements in a row (in our special case), a functional representation would be reasonable.

2.4 Quantum algorithms

2.4.1 Grover's Algorithm

Grover's algorithm is a quantum search algorithm. To search through a non-ordered list with N entries on a classical computer, one would have to go through individual entries of the list, requiring $O(N)$ operations. This can be sped up to $O(\sqrt{N})$ using a quantum circuit implementing Grover's algorithm.

Suppose we are searching through a list of N elements and assume there are M solutions to the search. To make the problem simpler, we consider searching index corresponding to the elements rather than the elements themselves. An index running from 0 to $N-1$ has been assigned to each element. The key object in Grover's algorithm is the quantum *oracle*, which, in the abstract sense, has the ability to *recognise* the solution states without *knowing* them. The oracle marks the solution states by flipping the sign of the state. Let $|x\rangle$ be one of the basis states and let $f(x) = 1$ if $|x\rangle$ is a solution state and $f(x) = 0$ if it is not a solution. The oracle performs the following linear operation (denoted as O):

$$|x\rangle \xrightarrow{O} (-1)^{f(x)} |x\rangle \tag{31}$$

What needs to be done now is to maximise the probability of observing one of the solution states. This cannot be achieved by re-applying the oracle right away, as this would undo the marking. Grover designed an algorithm to achieve this effect, and it is known as the Grover's diffusion operation. The procedure of the algorithm is as follows:

1. Apply the oracle O
2. Apply the Hadamard operation on all qubits $H^{\otimes n}$
3. Perform a phase shift of -1 on every state of the computational basis except $|0\rangle$:

$$|x\rangle \quad \longrightarrow -(-1)^{\delta_{x0}} |x\rangle \tag{32}$$

4. Apply the Hadamard operation on all qubits again $H^{\otimes n}$
5. Repeat step 1 to 4 for a certain number of times to maximise the probability of the solution states

Step 2 to step 4 is also known as the *inversion about mean* operation. Mathematically, this iteration can be written compactly as:

$$G = (2 |\psi\rangle \langle\psi| - \mathbb{I}) O. \tag{33}$$

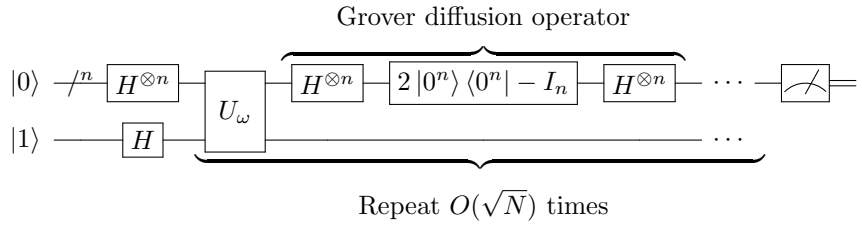

Figure 1: Circuit of Grover's Algorithm[1]

Fig. 1 shows a schematic circuit diagram for Grover's algorithm.

To determine the number of times the diffusion operation should be applied, we need to first Geometrically, the iteration performs a rotation of the state vector $|\Psi\rangle$ towards the vector representing a uniform superposition of the solution states on the plane spanned by the

$$|\alpha\rangle \equiv \frac{1}{\sqrt{N-M}} \sum_{\text{solutions}} |x\rangle \tag{34}$$

$$|\beta\rangle \equiv \frac{1}{\sqrt{M}} \sum_{\text{non solutions}} |x\rangle \tag{35}$$

Substituting these to the state vector gives:

$$|\Psi\rangle = \sqrt{\frac{N-M}{N}} |\alpha\rangle + \sqrt{\frac{M}{N}} |\beta\rangle \tag{36}$$

2.4.2 Shor's Algorithm

Fig. 2 shows a schematic circuit diagram for Shor's algorithm.

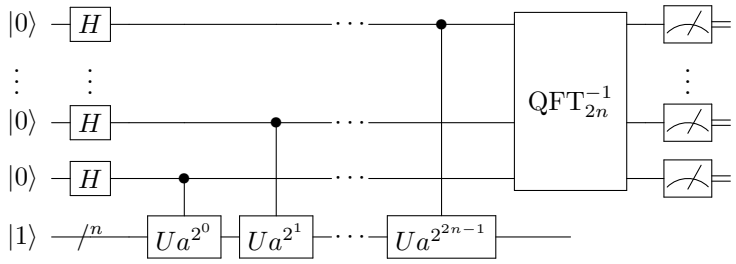

Figure 2: Circuit of Shor's Algorithm[2]

2.5 Building a quantum computer

3 Implementation

3.1 Project organisation

3.2 Development environment

3.3 Program structure

3.3.1 Overview

3.3.2 Matrix

3.3.3 Gates

Designing the gates is a challenging issue as there are multiple problems that addressed:

1. A design that allows different representations of a quantum gate, such as matrix representation and functional representation
2. A design which allows gates of d

3.3.4 Graphics User Interface

3.4 Program execution

4 Results

4.1 Grover's Algorithm

4.2 Shor's Algorithm

5 Discussion

5.1 Matrix or functional representation

5.2 Improvements and further steps

6 Conclusion

7 Appendix

References

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