Designing and Implementing Small Quantum Circuits and Algorithms

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ABSTRACT

It appears, in principle, that the laws of quantum mechanics allow a quantum computer to solve certain mathematical problems more rapidly than can be done using a classical computer. However, in order to build such a quantum computer a number of technological problems need to be overcome. A stepping stone to this goal is the implementation of relatively simple quantum algorithms using current experimental techniques.

This paper explores small scale quantum algorithms from two different perspectives. Firstly, it will be shown how small scale quantum algorithms can be tailored to fit current schemes for implementing a quantum computer. Secondly, I will review a simple model of computation, based on read-only-memory. This model allows the comparison of the space-efficiency of reversible error-free classical computation with reversible, error-free quantum computation. The quantum model has been shown to be more powerful than the classical model.

Categories and Subject Descriptors

F.1.1 [**Computation By Abstract Devices**]: Models of Computation

General Terms

Algorithms

Keywords

quantum algorithms, reversible quantum circuits

1. INTRODUCTION

Computers have become an indispensable component of the modern world. They take on a multitude of different forms in almost every aspect of our lives; from the familiar desktop personal computer, to the micro-chips located in electronic devices such as mobile phones, microwave ovens and even washing machines. The operation of all these computers can be explained in terms of classical mechanics[1]. However, quantum mechanics, not classical mechanics, is generally accepted as being a more fundamental physical theory.

What then, is the power of a computer which is governed by the laws of quantum mechanics? This is the question addressed by the field of quantum computation[2]. A complete answer to this question is not likely to be forthcoming in the near future. The analogous question for classical computation has been studied for almost a century, and yet the answer is still unknown. What has been shown, over the last decade, is that there are certain mathematical problems which a quantum computer can solve with fewer computational steps than a classical computer [22, 10]. However, building a quantum computer which can outperform any classical computer will not be a simple task. Although quantum mechanics holds true at the microscopic level, macroscopic objects are governed by classical mechanics. The transition between these two regimes is not well understood. A 'useful' quantum computer will need to be composed of thousands of qubits[3], and therefore will reside in the boundary region between the microscopic and the macroscopic.

This paper centers around *small scale* or *toy* quantum algorithms [26]. That is, algorithms which DO NOT solve mathematical problems faster than can be done classically. Rather, these algorithms act as a test-bed for quantum computation, allowing us to predict the problems which will arise as we gradually increase the 'size' of experimentally implementable quantum computers.

As stated in the abstract, the ideas presented in this paper can be broken down into two parts. Section 2 is dedicated to *hybrid quantum algorithms*. These are algorithms which utilize both the discrete quantum levels of a qubit, and the continuous levels of a quantum harmonic oscillator. In this section we describe a quantum version of a random walk on a line. Section 3 overviews the ROM-based model of com-

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[1]By this statement I mean the 'logical' operation of these computers is classical, of course to describe the workings of a semi-conductor transistor requires quantum mechanics.
[2]For an introduction to this field the interested reader might like to consult Nielsen and Chuang [17].
[3]A quantum bit or *qubit* is a two level quantum system.

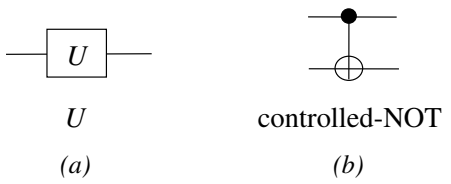

Figure 1: Circuit diagram for (a) an arbitrary one qubit gate, and (b) a controlled-NOT gate.

putation, highlighting the differences between the classical and quantum models. However, before delving into these areas, the following subsections will very briefly introduce the key concepts in quantum computation, and describe the basic principles of ion trap quantum computers.

1.1 Quantum Computation Basics

The model generally used to describe quantum computation is the quantum circuit model. Rather than manipulating series of bits using classical logic gates, the quantum circuit model is based upon the axioms of quantum mechanics. The basic unit of information in the quantum circuit model is the quantum bit, or qubit. A qubit is simply a two level quantum system. This means that a qubit is completely represented by a unit vector in a two dimensional Hilbert space. Denoting the two levels of this Hilbert space with the symbols $|0\rangle$ and $|1\rangle$, an arbitrary state of a qubit can be written as

$$|\psi\rangle \quad = \quad a|0\rangle + b|1\rangle, \tag{1}$$

where a and b are complex numbers, and normalization requires that

$$|a|^2 + |b|^2 \quad = \quad 1. \tag{2}$$

Quantum mechanics dictates that the Hilbert space associated with a string of qubits is the *tensor* product of the individual Hilbert spaces. Thus $2^m - 1$ complex numbers are required to completely describe an arbitrary state of m qubits.

Just as AND, NOT and FANOUT form a universal set for classical computation, one example of a universal set for quantum computation is the set containing arbitrary one qubit gates, and the controlled-NOT (CNOT) gate. The quantum circuit diagrams for these gates are depicted in Fig. 1. The operation of these gates can be completely described by giving their matrix representation in the computational basis,

$$U = \begin{bmatrix} e^{i(\delta-\alpha/2-\beta/2)}\cos\theta/2 & -e^{i(\delta-\alpha/2+\beta/2)}\sin\theta/2 \\ e^{i(\delta+\alpha/2-\beta/2)}\sin\theta/2 & e^{i(\delta+\alpha/2+\beta/2)}\cos\theta/2 \end{bmatrix} \tag{3}$$

and

$$\text{CNOT} \quad = \quad \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{4}$$

A quantum computation proceeds by initializing a string of qubits, which involves placing each qubit in the zero state,

$$|0\rangle_{n-1}|0\rangle_{n-2}\cdots|0\rangle_1|0\rangle_0. \tag{5}$$

It then proceeds by performing a series of U gates and CNOT gates. Finally the qubits are measured in the computational basis, obtaining an n-bit string. The quantum algorithm is a complete description of the sequence of U and CNOT gates to apply. For a given problem instance, the final measurement yields a bit string which, with finite probability, will correspond to the problem solution.

1.2 Ion Trap Quantum Computers

In the beginning of the introduction it was stated that the laws of quantum mechanics are generally accepted as being fundamental physical laws. We have also stated that the quantum circuit model obeys these laws. Why then, do we not already use quantum computers? The key problem is that quantum mechanics describes the evolution of *isolated* physical systems. It is the dual task of controlling the evolution of a physical system whilst trying to maintain a high degree of isolation which is extremely difficult to achieve experimentally. Considerable experimental effort is underway to develop physical systems which are suitable for quantum computation; in various forms ranging from gas to liquid to solid state. For a review of some schemes for implementing a quantum computer see the special issues on quantum computation in Fortschr. Phys. [8].

The hybrid algorithm discussed in the subsequent section is based on implementation in the ion trap quantum computer. Using ion traps for quantum computation was first suggested by Cirac and Zoller [5]. There are a number of groups world-wide who are performing quantum information experiments with ion traps, including the University of Aarhus, the University of Michigan, the University of Hamburg, IBM-Almaden, the University of Innsbruck, Kansai Advanced Research Center, Los Alamos National Laboratory, the Max-Planck Institute, the National Institute of Standards and Technology and Oxford University. For a nice review of the status and prospects of quantum information experiments with trapped ions I would suggest the recent papers by Hughes et al. [11] or Sackett [20].

As the name implies, an ion trap quantum computer requires the trapping of charged particles. It is impossible to trap a charged particle in free space using static electric fields. Thus, in the case of the linear Paul trap, the ions are confined using time-dependent radio-frequency electric fields [18, 9, 4, 23]. A schematic diagram of a linear Paul trap, taken from Sackett [20], is depicted in Fig. 2. The trap consists of four parallel rods. A radio-frequency voltage is applied to the continuous rods, while the segmented rods are held at a DC potential. This gives an oscillating field which is zero along a line between the rods. To provide axial confinement, a positive voltage is applied to the outer segments of the DC rods, while the inner segments are held at ground or a negative potential.

As the electric field oscillates rapidly compared to the frequencies of the ions' motion, the time-averaged effect on the ions can be described by a harmonic potential. Due to Coulomb forces, the ions are strongly coupled, with $3N$ different modes [12]. Each of these modes behaves as a quantum mechanical harmonic oscillator.

As single valence ions are generally used, their internal states are similar to those of a neutral hydrogen atom; thus there is a large number of states to choose from. The four key states required for quantum computation are depicted in Fig. 3. Two of the levels are selected as the $|0\rangle$ and $|1\rangle$ states.

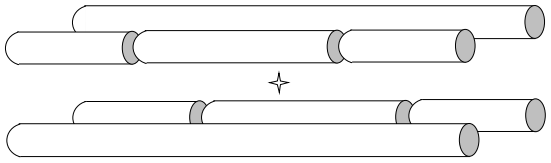

Figure 2: Schematic diagram of a linear Paul trap, consisting of four parallel rods. A radio-frequency voltage is applied to the continuous rods, while the segmented rods are held at a DC potential. The star indicates the position of the ion(s).

These levels ideally are not connected by a dipole transition; which means they have very low spontaneous emission rates, and are thus metastable. The $|p\rangle$ state is an unstable excited state which is used to initially prepare the ion in a known state. As the diagram indicates, it is possible for the electron to decay from $|p\rangle$ to $|1\rangle$ or $|0\rangle$. But by optically pumping the $|p\rangle \leftrightarrow |1\rangle$ transition, eventually the ion will be left in the $|0\rangle$ state with high probability. This procedure has been used to prepare ions with fidelities greater than 0.99 [20].

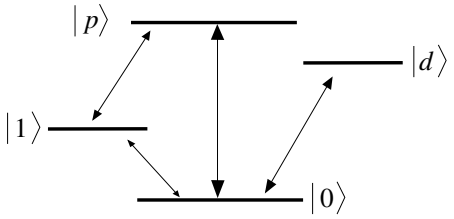

Figure 3: Electronic energy levels required for an ion qubit. States $|0\rangle$ and $|1\rangle$ are meta-stable states which store the quantum information. State $|p\rangle$ is used for optical pumping, required to prepare the ion in a known state. State $|d\rangle$ is used for detection.

As well as preparing the internal state of the ions it is also necessary to prepare the ions in the motional ground state. One of the mechanisms used to cool the ions to their ground state is known as sideband laser cooling [29, 19, 7]. Sideband laser cooling is accomplished by tuning a laser to the first red sideband. This is a frequency which is one unit of vibrational frequency below the atomic transition. Thus a transition of the form $|0, n\rangle \leftrightarrow |d, n-1\rangle$ is induced, where the zero denotes the internal ground state, the d denotes the detection state (see Fig. 3), and the n and $n-1$ represent phonon number states. Thus each excitation/decay cycle of the ion will remove approximately one quantum from the motional mode.

Single qubit operations are performed by coherently driving the $|0\rangle \leftrightarrow |1\rangle$ transition for a time t and with a phase ϕ, which in the interaction picture, results in the operation $R(\Omega t, \phi)$, where Ω is Rabi frequency for the transition and

$$R(\theta, \phi) = \begin{bmatrix} \cos(\theta/2) & e^{i\phi}\sin(\theta/2) \\ -e^{-i\phi}\sin(\theta/2) & \cos(\theta/2) \end{bmatrix}. \quad (6)$$

Couplings between the internal states of the ions and their motional states are achieved by applying red or blue sideband laser pulses similar to those applied during the cooling process [6, 14, 12].

Finally, near perfect detection of an ion can be accomplished by driving a transition between the states $|0\rangle \leftrightarrow |d\rangle$ (see Fig. 3). If the ion is in the $|0\rangle$ state then it will fluoresce brightly as the ion cycles between the two states. Whereas, if the ion is in the $|1\rangle$ state, no fluorescence will be observed. The number of photons emitted by the bright state can be more than 10^5, thereby creating detection efficiencies greater than 99% [15, 21, 3].

2. HYBRID QUANTUM ALGORITHMS

One might wonder if the term small scale is applicable when used in conjunction with a continuous quantum system, which spans an infinite Hilbert space. In practice, however, the size of the Hilbert space is limited by experimental considerations, such as the precision to which a measurement can be made, or the amount of energy which can be supplied to a system.

There are several reasons why we might want to initially implement quantum algorithms which utilize a continuous quantum variable. Firstly, it gives us access to a Hilbert space which, though not infinite, is far larger than we can currently create using qubits alone. Another reason is that certain mathematical problems are easily described in terms of a single many level system rather than a combination of two level systems. However, our main reason is to attempt to fully utilize the natural dimensionality of the ion trap quantum computer.

We describe below the implementation of a quantum analog of the random walk on a line [16]. The tailoring of this algorithm to an ion trap was initially described in [27].

2.1 Quantum Walk

Recently, several groups have investigated quantum analogues of random walk algorithms, both on a line [16] and on a circle [1]. It has been found that the quantum versions have markedly different features to the classical versions. Namely, the variance on the line, and the mixing time on the circle increase quadratically faster in the quantum versions as compared to the classical versions. Here, I review a scheme to implement the quantum random walk on a line in an ion trap quantum computer. With current ion trap technology, the number of steps that could be experimentally implemented will be relatively small. However, it should be possible to implement enough steps to experimentally highlight the differences between the classical and quantum random walks, providing an important proof of principle. In the limit of strong decoherence, the quantum random walk tends to the classical random walk. By measuring the degree to which the walk remains 'quantum', this algorithm could also serve as an important bench-marking protocol for ion trap quantum computers.

Random walks can take many different forms, starting from the simple discrete random walk on a line, to random walks on graphs, to continuous time random walks, such as brownian motion. In this paper we are only considering discrete time, discrete space, random walks on a line. Imagine a person standing at the origin of a line with a coin in their hand. They flip the coin, and if it comes up heads, they take a step to the right, if it is tails, they take a step to the left (all steps are of a fixed size). They then repeat this procedure, flipping the coin, and taking a step based on the

result. The probability, $P_N(d)$, of being in a position d after N steps is

$$P_N(d) = \frac{1}{2^N}\left(\begin{array}{c} N \\ \frac{d+N}{2} \end{array}\right), \quad (7)$$

where $P_N(d)$ is defined on the set $d \in \{-N, -N+2, \ldots, N-2, N\}$ and the round brackets denote the combination of two integers, $\left(\begin{array}{c} n \\ r \end{array}\right) = {}^nC_r$. The non-zero elements of the distribution are simply terms from Pascal's triangle, divided by the appropriate factor of two.

Now let us consider a quantum version of the walk on a line. The first modification we can make is to replace the coin with a qubit. In this section we shall be representing the two levels of the qubit with the states $|\downarrow\rangle$ and $|\uparrow\rangle$ rather than $|0\rangle$ and $|1\rangle$. If we start with the qubit in the down state, and apply a Hadamard operation, we get an equal superposition of up and down,

$$H|\downarrow\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{1}{\sqrt{2}}|\downarrow\rangle, \quad (8)$$

remembering that

$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \quad (9)$$

If we were to measure the qubit, and step left or right depending upon the result, we would obtain exactly the classical walk described above. Now, rather than a person holding a coin, suppose we have a particle, whose motion is confined to one dimension. We can now treat the particle as a quantum system, and perform the quantum walk as follows. During each iteration, we apply the Hadamard operation, followed by the operation which steps right if the qubit is down, and steps left if the qubit is up. That is, we apply the operator

$$\hat{U} = e^{i\hat{p}Z}H, \quad (10)$$

where $\hat{p}$ is the momentum operator of the particle confined to one dimension, and Z is the Pauli-z operator acting on the qubit. Thus, if we initially start the system with the qubit in the down state and the particle at the origin,

$$|\Psi_0\rangle = |0\rangle|\downarrow\rangle, \quad (11)$$

applying Eq. (10) results in the state

$$\begin{aligned} |\Psi_1\rangle &= \hat{U}|\Psi_0\rangle \\ &= e^{i\hat{p}Z}H|0\rangle|\downarrow\rangle \\ &= \frac{e^{i\hat{p}Z}}{\sqrt{2}}(|0\rangle|\downarrow\rangle + |0\rangle|\uparrow\rangle) \\ &= \frac{1}{\sqrt{2}}(|1\rangle|\downarrow\rangle + |-1\rangle|\uparrow\rangle). \end{aligned} \quad (12)$$

Therefore, the state of the system after N steps is

$$|\Psi_N\rangle = \left(e^{i\hat{p}Z}\right)^N|\Psi_0\rangle, \quad (13)$$

where $|\Psi_0\rangle$ is the initial state of the system. The mean of the distribution produced by this quantum random walk is not necessarily zero. It is dependent upon the initial state of the qubit. For example, choosing the initial state of the qubit to be down gives a non-zero mean after the second step. For the remainder of this paper, we shall only be considering the distribution created with the initial qubit state $\frac{1}{\sqrt{2}}|\downarrow\rangle + \frac{i}{\sqrt{2}}|\uparrow\rangle$ which has a mean of zero for all values of N,

$$|\Psi_0\rangle = \frac{1}{\sqrt{2}}|0\rangle(|\downarrow\rangle + i|\uparrow\rangle). \quad (14)$$

The non-zero elements of this distribution are no longer simply terms from Pascal's triangle which arose in the classical case. The deviations from the classical distribution are caused by quantum interference effects.

The ion trap provides a convenient setting for implementing this walk, as it contains the required discrete and continuous quantum variables. For the remainder of this chapter we shall be discussing implementations based on a single $^9Be^+$ ion, confined in a coaxial-resonator radio frequency (RF)-ion trap, as described in [14] and references therein.

The preparation involves laser-cooling the ion to the motional and electronic ground state, $|0\rangle|\downarrow\rangle$, as described in [13]. A sequence of four Raman beam pulses are then applied [14] to create the state $(|\alpha\rangle|\downarrow\rangle + |-\alpha\rangle|\uparrow\rangle)/\sqrt{2}$, where $|\alpha\rangle$ denotes the coherent state of the oscillator. The first pulse is a $\pi/2$-pulse which creates an equal superposition of $|0\rangle|\downarrow\rangle$ and $|0\rangle|\uparrow\rangle$. A displacement beam is then applied which excites the motion correlated to the $|\uparrow\rangle$ internal state. The third pulse is a π-pulse which exchanges the internal states, and finally the displacement beam is applied again. The combined action of the four pulses is to effectively perform the operator $\hat{U}$, defined in Eq. (10). The quantum random walk on the line is accomplished by repeating this sequence of pulses N times. Fig. 4 contains the Wigner function obtained by tracing over the internal degree of freedom after five steps of the quantum random walk algorithm.

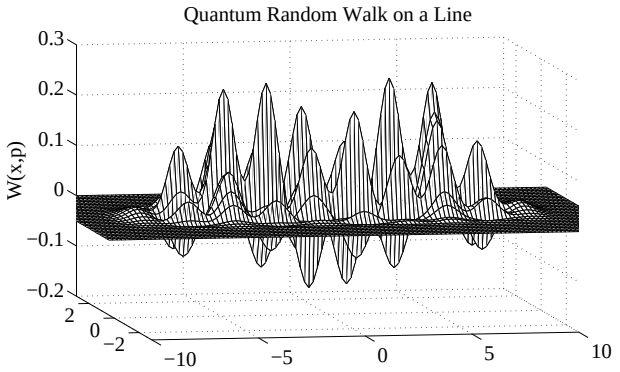

Figure 4: Wigner function of the particle after five steps of the quantum random walk on the line. (The electronic level of the ion has been traced over.)

In current ion trap experiments there are a number of sources of decoherence. The largest source in many experiments is anomalous heating of the lower vibrational modes of the ions. The theory behind this heating is not well understood. Therefore, in this section we neglect this source of decoherence, and instead concentrate on the decoherence of the electronic levels of the ion.

Decoherence of the electronic levels of the ion during the application of the algorithm has the effect of gradually transforming the quantum random walk to the classical random walk. Rather than considering this to be a negative effect, we can measure the degree to which the ion is acting as a quantum variable rather than a classical variable, and

thereby effectively measure the level of decoherence in the ion trap.

The scheme for measuring the random walk utilizes similar operators to those employed in the application of the algorithm. After applying the random walk sequence for some number of steps, the internal state of the ion is decoupled from the motional state by an appropriate Raman pulse. An effective operator such as $\exp(i\hat{p}Y)$ is applied, where Y is the Pauli-y operator. Before finally measuring the internal state of the ion. Thus we are using the internal state of the ion to supply us with information about the motional state. Suppose we decouple the internal state from the motional state by measuring whether the ion is in the state $|\uparrow\rangle$ or $|\downarrow\rangle$. We then apply the operator

$$\hat{M}^{\pm} \quad = \quad e^{\pm i\hat{p}Y}. \tag{15}$$

The positive Hamiltonian is applied upon obtaining the results $|\uparrow\rangle$, whilst the negative Hamiltonian is applied otherwise. Finally, we again measure the internal state of the ion. This last measurement result yields information about the spread of the probability distribution associated with the random walk [27].

3. ROM-BASED COMPUTATION

It is well known that the measurement of a qubit can yield a maximum of one bit of information. This does not mean, however, that a single qubit and a single bit have the same computational power. This section introduces a model of computation based on *read only memory* (ROM), which allows us to compare the space-efficiency of reversible, error-free classical computation with reversible, error-free quantum computation. This model, and the results presented in this section were developed by coauthors and myself in Travaglione et al. [28] and experimentally implemented in [24].

In this section we consider mappings between strings of boolean variables (bits) of the following form,

$$u_1 u_2 \ldots u_j \underbrace{00\ldots0}_{n \text{ (qu)bits}} \quad \stackrel{F}{\longrightarrow} \quad u_1 u_2 \ldots u_j f_1 f_2 \ldots f_n, \tag{16}$$

where each $u_i \in \{0,1\}$ and each $f_i \in \{0,1\}$. It is evident from Eq. (16) that the first j bits have the same initial and final values; however in our model we shall require that the values of the first j bits are also not altered during any of the steps of the computation, so we can consider them to be *read-only memory* or ROM bits. Each of the last n bits are mapped to zero or one, depending on the values of the ROM bits. Therefore we can think of each of these n bits as *writable* bits, whose final value is a boolean function of the ROM-bits,

$$f_i(u_1, u_2, \ldots, u_j) \quad : \quad \mathbb{B}_2^j \rightarrow \mathbb{B}_2 \quad i \in \{1, 2, \ldots, n\}, \tag{17}$$

where $\mathbb{B}_2^j$ denotes a binary string of length j.

In the classical case, a given function f_i is generated by a sequence of arbitrary classical *reversible* gates acting on the n writable bits. Additionally, any of these gates can be applied conditionally upon the value of *one* of the j ROM bits. We are using only reversible gates to preserve the number of writable bits.

In the quantum case, arbitrary quantum gates can be applied to the n qubits, and once again any of these gates can be applied conditionally upon the value of *one* of the j ROM bits. However, it should be remembered that each of the f_i are boolean expressions; thus whilst the qubits can exist in superpositional states during the computation, at the conclusion they must be in a computational basis state. This means that the entire computation (including measurement) is deterministic and reversible, as measuring the n qubits at the end of the computation will have no effect on their state. Intermediate measurements can be made in neither the quantum or classical models, as the storing of the measurement result would be effectively expanding the workspace.

Just as in conventional quantum circuit theory, we can use circuit diagrams to represent ROM-based computations. As is standard in quantum computational circuit diagrams, the writable (qu)bits will be represented as horizontal lines, whose states change as various gates are applied from left to right. The ROM bits will be depicted above the circuit diagram, with a line from a ROM bit to a gate implying that this gate is applied only if the ROM bit has value one. Fig. 5 contains an example of a ROM computation circuit diagram. This diagram depicts the computation

$$u_1 u_2 u_3 |0\rangle|0\rangle \quad \stackrel{F}{\longrightarrow} \quad u_1 u_2 u_3 |f_1\rangle|f_2\rangle, \tag{18}$$

where

$$\begin{aligned} |f_1(u_1, u_3)\rangle \quad &= \quad |u_1 \oplus u_3\rangle \quad \text{and} \\ |f_2(u_1, u_2)\rangle \quad &= \quad |u_1 \oplus u_1 u_2\rangle. \end{aligned} \tag{19}$$

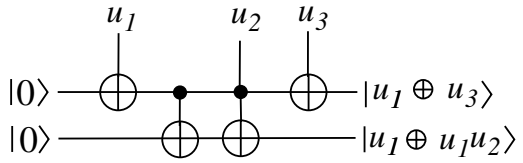

Figure 5: An example of a ROM-based circuit diagram. The variables at the top of the diagram are the ROM bits.

There are $2\hat{}(n2^j)$ Boolean functions from j bits to n bits. We shall define as *universal* a ROM-based computer which is capable of calculating all of these functions.

THEOREM 1. *A ROM-based* quantum *computer with one writable qubit is universal.*

For brevity, we omit the proof of this theorem, which can be found in [28].

On the other hand, a ROM-based classical computer with one writable bit will *not* be universal. This can be seen as a consequence of theorem 5.2 from [25], which states that there exist invertible functions of order n which cannot be obtained by composition of generalized Toffoli gates of order strictly less than n.

Now consider a ROM-based classical computer with two writable bits. It is possible to deduce that this will be universal using Lemma 7.3 from Barenco et al. [2]. Thus we have the following theorem:

THEOREM 2. *A ROM-based* classical *computer with two writable bits is universal.*

These two theorems imply that the a quantum computer is more space efficient within this model.

4. CONCLUSIONS

We have shown how certain simple quantum algorithms can be tailored to fit current experimental schemes. In particular, we have reviewed an implementation scheme for a quantum random walk using ion trap technologies. At this point it is unclear whether discrete quantum walks will have any useful algorithmic applications. However, they can provide an important tool for exploring the effects of decoherence within an ion trap quantum computer. We have also shown that quantum computation is more space efficient within the ROM-based model of computation.

In conclusion, although large scale quantum computers may not be built for many years to come, this paper has pointed to some small scale algorithmic tasks which can be investigated using current experimental techniques. These small scale quantum algorithms allow us to analyze essential aspects of quantum computation; such as decoherence rates and minimum resource requirements.

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