Where to quantum walk

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31st May 2011

Abstract

Quantum versions of random walks have diverse applications that are motivating experimental implementations as well as theoretical studies. However, the main impetus behind this interest is their use in quantum algorithms, which have always employed the quantum walk in the form of a program running on a quantum computer. Recent results showing that quantum walks are “universal for quantum computation” relate entirely to algorithms, and do not imply that a physical quantum walk could provide a new architecture for quantum computers. Nonetheless, quantum walks used to model transport phenomena in spin chains and biomolecules broaden their scope well beyond algorithms, and reopen the question of when a physical implementation might provide useful computational outputs. In this article we determine the conditions under which a physical quantum walk experiment could provide useful results beyond the reach of classical computation.

1 Introduction

Quantum versions of random walks were introduced in the late 80s by Gudder [1] and Aharonov, Y et al. [2]. Early work by Grossing and Zeilinger [3] and Meyer [4, 5, 6] focused on the more general case of quantum cellular automata. The first application to quantum algorithms was by Farhi and Gutmann [7] using a continuous time quantum walk. Aharonov, D et al. [8] and Ambainis et al. [9] described discrete time quantum walks from an algorithmic perspective, starting a decade of increasingly intense study of their applications and properties. In the simplest setting of a line or a Cartesian lattice, on which the walker hops between integer sites, a quantum walk spreads quadratically faster than a classical random walk. This provides the speed up in many quantum walk algorithms, e.g., for basic searching as presented by Shenvi et al. [10]. For a recent review of quantum walk searching see Santha [11]. Exponential speed up has been proved for crossing a hypercube by Kempf [12, 13] more efficiently than a classical random walk, and Childs et al. [14] proved a continuous time quantum walk can find its way through a particular “glued trees” graph exponentially faster than any classical algorithm. On the other hand, the phenomenon of Anderson localization [15] of quantum particles is well-known, and has been related to continuous time quantum walks by Keating et al. [16]. Studies by Krovi and Brun [18, 17, 19] confirm this extends to the discrete time setting, and highlight the importance of symmetry in the behaviour of quantum walks. Štefaňák et al. [20, 21] have characterized the localization of unbiased quantum walks on

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regular lattices, showing how it depends on the topology of the lattice, the coin operator and chosen initial state.

Quantum walks provide useful models of physical phenomena, such as quantum state transfer in spin chains as introduced by Bose [22] and reviewed by Kay [23], or energy transport in biomolecules (Mohseni et al. [24]). Perfect quantum state transfer can be achieved for particular configurations (reviewed in Kendon and Tamon [25]), of interest for building quantum wires in quantum computers. Highly efficient transport can be obtained by using imperfect quantum walks where the amount of decoherence is tuned to optimise the quantum walk properties [26, 27].

Experimental implementations of quantum walks were proposed from the beginning [2], the first photonic realisation [28] was recognised retrospectively by Sanders et al. [29]. Implementation using atoms trapped in an optical lattice as proposed by Dür et al. [30] was recently performed by Karski et al. [31]. Their atoms maintained full quantum coherence for up to ten steps, with decoherence degrading the walk to classical spreading after 25 steps. A quantum walk on four sites, as a computation in a three qubit NMR quantum computer, was implemented by Ryan et al. [32], who performed state tomography on all eight steps of the periodic dynamics and also applied decoherence to demonstrate the transition to a classical random walk. Recent work by Schreiber et al. [33] achieved 28 fully coherent steps of a photonic quantum walk, mapping the position to time delays in the photon propagation provided by fibre loops. Using time delays to encode the locations allows a single set of components to be used for all sites and steps of the quantum walk; the detection system records the time of arrival of the photons with sufficient accuracy to distinguish all the encoded locations. They also demonstrated 11-step walks with fully controlled decoherence of three different types, static disorder leading to Anderson localisation, fast fluctuations returning the walk to classical behaviour, and slow fluctuations that produce even faster spreading when averaged over many walks. Photonic quantum walks can also be performed in substrates containing the sites. Broome et al. [34] used separate calcite crystals for each step of the walk, with the position mapped to the displacement of the walker across the crystal. Coupled photonic waveguides for quantum walks were first employed by Perets et al. [35] performing a continuous time quantum walk across 100 lattice sites. Multiple correlated photons can easily be injected into such devices [36]. However, these waveguides contain a fresh set of sites for each step of the walk, a significant extra resource compared to designs that reuse the same components.

Recent work by Childs [42] proving that quantum walks are “universal for quantum computation” has renewed interest in their role in quantum information. However, it is important to direct research efforts in the most effective directions. This paper places this important result in context, and explores the computational potential of quantum walk experiments. A brief overview of quantum walks is given in the next section, followed in section 3 by a description of how quantum walks are used as a tool for quantum algorithms. In section 4 the limitations of classical simulations of quantum walks are described, and the possibilities for usefully expanding beyond these limits with quantum walk experiments are explored. Conclusions are summarised in section 5.

2 Quantum Walks

Like classical random walks, quantum walks have both discrete time [2, 37, 8, 9], and continuous time [7] versions. We briefly review the simplest walk on a line, since many experiments have focused on this instance. A discrete quantum walk on a line is defined in direct analogy with a classical random walk, where the walker steps one unit forward or back based on the outcome of a random
coin toss. The quantum walker has a quantum coin that will in general be in a superposition, so the quantum walker ends up in a superposition of positions on the line. However, the coin toss is not random, since pure quantum dynamics need to be unitary, but if measured, the outcome of the measurement would be random, like the classical coin. We define a two-dimensional quantum coin with basis states $|\pm 1\rangle$ and label the position basis states $|x\rangle$ by the integer location on the line $x$. The evolution of the walk is governed by a coin operator that acts on the quantum coin at each step of the walk. The simplest choice is the Hadamard coin operator, 

$$C_2^{\text{(Had)}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{1}$$

Varying the phase $\beta$ in the initial coin state $|c_0\rangle$:

$$|c_0\rangle = \sqrt{b}|-1\rangle + e^{i\beta}\sqrt{1-b}|+1\rangle, \tag{2}$$

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where $b$ is the bias in the initial state, and $\beta$ is the relative phase between the two components, produces outcomes with varying skewness \[^{[38]}\]. After “tossing” the coin with the coin operator, the particle moves to adjacent positions conditioned on the coin state

$$S|-1, x\rangle = |-1, x - 1\rangle$$
$$S|+1, x\rangle = |+1, x + 1\rangle. \tag{3}$$

Here we have written $|c, x\rangle \equiv |c\rangle \otimes |x\rangle$ for combined basis states. One step of the quantum walk is produced by the unitary operator $U = S(C \otimes \mathbb{I}_x)$. A quantum walk of $T$ steps starting from an initial state $|\psi_0\rangle$ is thus

$$|\psi_T\rangle = U^T|\psi_0\rangle. \tag{4}$$

The position probability distribution of a quantum walk on a line is by now well-known, the time evolution over 100 steps with a Hadamard coin operator and initial state of $\frac{1}{\sqrt{2}}(|+1, 0\rangle + i|-1, 0\rangle)$ is shown in figure 1. The double-peaked spreading expands at a linear rate, giving a quadratic speed up over the $\sqrt{T}$ spread of the binomial distribution produced by a classical random walk on the line.

The continuous time quantum walk on a line is even simpler. The quantum walker has a transition probability $\gamma$ per unit time to hop left or right to neighbouring positions. This can be expressed as a Hamiltonian

$$H = \sum_{x=-\infty}^{+\infty} \gamma \{|x - 1\rangle\langle x| + |x + 1\rangle\langle x|\}. \tag{5}$$

The quantum walk evolves according to the Schrödinger equation,

$$i\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle, \tag{6}$$

with formal solution

$$|\psi(t)\rangle = \exp\{-iHt\}|\psi(0)\rangle, \tag{7}$$

where $|\psi(t)\rangle = \sum_x a_x(t)|x\rangle$ and the $\{a_x(t)\}$ are complex numbers with normalisation $\sum_x |a_x(t)|^2 = 1$. The time evolution is very similar to the discrete time quantum walk on the line depicted in figure 1 with the same quadratic speed up over its classical counterpart.
Figure 1: Probability distribution for a quantum walk on the line over 100 steps showing evolution of system, using a Hadamard coin, equation (1), and a symmetric initial state \((|+1,0\rangle + i|-1,0\rangle)/\sqrt{2}\). Only positions with non-zero probability of occupation are shown, since odd positions are unoccupied at even time steps and vice versa.

Discrete and continuous quantum walks have been solved analytically on regular structures and their asymptotic scaling described in detail \([9, 8, 39]\). Differences in their behaviour compared with classical random walks are also found when there are absorbing boundaries \([38]\). Both discrete and continuous time quantum walks generalise straightforwardly from the line to arbitrary connected structures (graphs), usually described by their adjacency matrix \(A\). An edge between sites \(x\) and \(y\) is represented by the \(xy\)th entry in \(A\) being one, with zeros elsewhere. For the continuous time quantum walk, the Hamiltonian becomes \(H = \gamma A\). The discrete time walk needs a mapping between the coin states and the choice of edge at each sites \([40, 41]\).

3 Algorithmic quantum walks

Algorithmic uses of quantum walks are always binary encoded in the quantum computer. Without this, the efficiency gains they provide would be negated. Binary encoded means that the position of the walker is stored as a superposition of binary numbers in a qubit register. For simplicity, we will illustrate this for the discrete time quantum walk on the line, but it is easily generalised to any labeled set of positions. The state of the quantum walker after \(T\) steps,

\[
|\psi_T\rangle = U^T|\phi_0\rangle = \sum_{c,x} a_{c,x}(T)|c,x\rangle,
\]  

(8)
with complex amplitudes \( a_{c,x}(T) \) satisfying \( \sum_{c,x} |a_{c,x}(T)|^2 = 1 \), can equally well be interpreted as the superposition state of a quantum register where \( x \) written in binary is the pattern of zeros and ones, and \( c \) is an extra bit recording the state of the coin. For a quantum walk of \( T \) steps, the furthest it can travel is to \( x = \pm T \), so we need \( \lceil \log_2(2T + 1) \rceil \) qubits, plus one more for the coin, in our quantum register. A quantum walk of a million steps thus requires just 22 qubits. The continuous time quantum walk needs to be discretised for quantum computation and this can be done efficiently, see Childs et al. [14], using similar resources to a discrete time walk [41].

3.1 Universality of quantum walks

Recent work by Childs [42] proving that “quantum walks are universal for quantum computation” uses the correspondence between Hamiltonians and continuous time quantum walks to prove that any quantum algorithm can be recast as a quantum walk algorithm. To ensure the algorithm is efficient, the Hamiltonian must be “suitably sparse” [14, 43, 44], as explained below. The discrete time quantum walk has also been shown to be universal in the same sense [45], using a similar mapping between the circuit model of quantum computing and a quantum walk on a graph derived from the circuit. A simple example is illustrated in figures 2 and 3. Comparison of these figures shows clearly that the graph on which the quantum walk takes place is exponentially larger than the quantum circuit.

A fully general Hamiltonian over \( n \) qubits has \( 2^n \times 2^n \) terms, requiring an exponential amount of information to describe it. It therefore cannot represent an efficient quantum computation. To obtain an efficient quantum computation, the graph on which the quantum walk takes place must have a description that is logarithmic in the number of sites – this corresponds to it being “suitably sparse”. This is clearly the case for the graph in figure 3 since it has been derived from the circuit in figure 2. If the description of the classical structure of sites on which the quantum walk takes place is inconveniently large, the job of storing and accessing the description is given to an oracle, as in Childs et al. [14]. Such oracles are a theoretical computer science concept, not intended to be implemented in an actual computation or experiment. The proof by Childs that quantum walks are universal for quantum computation allows the mathematics of quantum walks to be applied more generally to theoretical computer science, potentially facilitating advances in both areas. It does not suggest that a physical quantum walk on a structure like that of figure 3 is an efficient way to build a general purpose quantum computer.
4 Comparing classical and quantum

Although algorithmic uses of quantum walks do not require physical quantum walk experiments, this still leaves the possibility that a quantum walk experiment could provide useful computation of quantum walks themselves. At first sight this appears to blur the distinction between computation and experiment. We will avoid circularity (and philosophical issues) by taking a computation in this context to mean starting from a mathematical model – in this case the quantum walk dynamics as described by equations (4) or (7) – and calculating properties of it. A quantum walk experiment that accomplishes this must thus be set up to match the particular quantum walk under study. This requires well-characterised experimental apparatus to provide confidence it is really doing the correct quantum walk. We will, of course, test our experiment by performing simple quantum walks for which the outcomes are already known. In other words, we do an experiment to check our apparatus matches the mathematical description we have for it, then we do the experiment to perform the quantum walk computation we really want. The extrapolation is not guaranteed to work, but similar uncertainty is inherent in numerical simulation. The computer code used to do a classical computation of a quantum walk may have errors, and similar tests using known quantum walks are done to reduce this possibility.

The reason why a quantum walk experiment could be efficient enough to be computationally useful is because it avoids much of the overhead created by translating the quantum walk dynamics into numbers and elementary gate operations in a computer, be it quantum or classical. This can only give us an advantage for particular cases, because the exponential saving in memory by encoding the position as a binary number in a quantum computer will always win eventually as the quantum walk gets larger and longer. But we don’t yet have large quantum computers, the most powerful general purpose computational devices we have are classical computers. So we need to compare quantum walk experiments with current classical computational capabilities.
4.1 Classical computational limits

Classical numerical simulation of a quantum walk is a straightforward evaluation of equation (4) or (7), or their generalisations for different graphs. In high-level computational environments, such as Matlab, it takes only a few lines of code. As with any full simulation of a quantum system, we need to store and manipulate all of the complex amplitudes $a_{c,x}(t)$ describing the wavefunction, as given in equation (8). Each amplitude requires two floating point numbers (real and imaginary parts). Using 32 bits (4 bytes) for each floating point number, we can store $2^{27}$ amplitudes in 1 Gbyte of memory. For comparison, a new desktop computer in 2011 probably has around 4 Gbyte of memory in total. As already noted, a quantum walk on the line of a million steps needs only 22 qubits, described by $2^{22}$ amplitudes, which requires about 4Mbyte of memory, and this computation is quick and easy on a desktop computer. One of the largest simulations of a quantum system to date was not of a quantum walk, but of 36 qubits, requiring $2^{36}$ amplitudes. De Raedt et al. [46] employed many computers in parallel with a combined total of 1 Terabyte of memory – a new desktop computer in 2011 probably has a hard disk of this size. Each additional qubit doubles the memory required, so it is easy to appreciate that a quantum computer of just 40 logical qubits could outperform any classical computer.

4.2 Experiments and scaling

However, quantum walks are not qubit systems, a physical quantum walk on a line of a million steps (easily computed on any desktop computer) covers about two million sites, which is a significant experimental challenge, whether the sites are spatial as in Karski et al. [31] or mapped to time delays as in Schreiber et al. [33]. It is not possible to save resources by having a “quantum substrate” that stores the sites in some sort of superposition. This would amount to having a “quantum hash table”, which was proved impossible by Nayak [47]. The quantum coherence required for a million steps is even more challenging than building the substrate, but higher dimensional walks cover the ground faster. For a two-dimensional lattice, two million sites is $1414 \times 1414$, and supports only 706 time steps. In three dimensions, two million sites is roughly $125^3$, taking just 62 steps to fill. This is not far from the number of steps in recent experimental quantum walks on a line. The big difference is that you need a six-dimensional coin for a walk on a 3D lattice, although this is not a problem in principle, see Hamilton et al. [48] for a proposal utilising orbital angular momentum of photons. The most recent experiments have achieved quantum walks on tens [31, 33], or at most a hundred sites [35], so there is some way to go before the classical computational capabilities of millions of sites can be beaten.

4.3 Random substrates

Quantum walks on regular structures are easier to implement because the symmetry simplifies various aspects of the task. These symmetries also simplify the classical computation, and in many cases facilitate analytic solution too. A more difficult problem is quantum walks on disordered systems, such as percolation lattices. A recent numerical study in Leung et al. [49], of 1D and 2D percolation lattices probed the average behaviour over many random percolation lattices. On a line they studied 10,000 steps, about $2^{14}$ locations, with around 5000 repetitions over different percolations. In two dimensions, they ran simulations for 140 time steps, $281 \times 281$, which is roughly $2^{16}$ lattice sites. On a workstation, it took a week to do 5000 repetitions with different percolation lattices. The task that took most time was actually generating the pseudo-random
numbers needed to create each percolation lattice. To carry out a similar calculation with a quantum walk experiment requires a way to produce random percolation lattices for the quantum walk to take place on. Generating the randomness is not difficult in itself, any laboratory has sufficiently random sources of noise. Arranging for the randomness to create a percolation lattice for the quantum walk requires a new experimental design.

4.4 Strong versus weak simulation

There is a further issue that needs to be considered when comparing quantum and classical computations of quantum walks. The classical computation as described in this article gives as output the values of all of the complex amplitudes \( a_{c,x}(T) \) defining the quantum state. This is known as “strong simulation” \([50]\). Experimental quantum walks provide just one output, usually a location at which the quantum walker ended up. Further information can only be obtained by performing many repetitions of the experiment, to build up the probability distribution. Classical simulation that is strictly equivalent to this is known as “weak simulation”. It uses less resources per run, but similarly requires many repetitions to obtain more information. With clever algorithmic or experimental design, it may be possible to perform a final measurement that yields more useful information directly (the mean or standard deviation, perhaps). With photonic quantum walks in particular, it may be so easy to perform many repetitions that this issue does not constitute a problem, even for producing sufficient statistics to construct the whole probability distribution.

4.5 Decoherence

As well as perfect quantum walks, it is also important to understand what happens when imperfections affect the quantum walk dynamics. While some simple models of Markovian noise can be solved analytically, many cases require numerical simulation \([51]\). Using models in which the noise is provided by nonlinear operators in a standard master equation, the quantum state is now represented by a density matrix, and the classical simulations require roughly the square of the resources necessary for a pure quantum state. This reduces the size of the largest practical classical simulation of a quantum walk down to around \(2^{12}\) sites on a workstation. This is only \(64^2\) or \(16^3\), so the number of steps, even in two dimensions, is comparable with current experiments. In a classical computation, individual control of the decoherence at each site and step can be done easily, the extra resources being proportional to the size of the description of the required controls. In an experiment, arbitrary controls add significant complexity to the design, see Schreiber et al. \([33]\) for example.

4.6 Multiple walkers

There is one important case where a physical implementation can win even sooner over classical computers: when there are multiple interacting walkers. Multiple non-interacting walkers only add particle statistics (for indistinguishable walkers), they live in a predictable subspace of the full Hilbert space that can be simulated as efficiently with classical computers as single walkers. Analytical and numerical study of non-interacting multiple walkers are not as advanced as for single walkers, but many cases of interest are analytically tractable, \([52, 53]\). However, when an interaction is added between walkers occupying the same site, the resources required for classical simulation grow quickly. With \(m\) walkers on \(L\) locations, the full Hilbert space is of size \(L^m\). The
exponential growth in the size of the Hilbert space is the same as for qubits, hence the size of such
classical simulations is limited to $L^m < 2^{40}$ for current capabilities. Multiple interacting quantum
walkers have been studied from the earliest days of quantum walks: they are quantum cellular
automata. They have been proved capable of universal quantum computation, for a review of their
significance and properties, see [54]. Quantum cellular automata are particular suited to optical
lattice experiments. A scheme with two coupled walkers has been proposed by Ahlbrecht et al.
[55], as a first step in this direction.

5 Conclusions

A Hilbert space of size $2^{40}$ corresponding to 40 spin-1/2 systems is beyond current classical ca-
pabilities. Quantum walks with a single walker and a Hilbert space of this size can be performed by
a qubit quantum computer with 40 qubits, but a physical quantum walk of this size would require
around $10^{12}$ sites to be provided, a more challenging experiment than a 40 qubit quantum com-
puter. Ion trap and optical lattice experiments already trap many more than 40 ions and atoms,
but not yet with the dynamical control required for general operations.

When making the comparisons it should be remembered that classical simulations can provide
information about the complete quantum wavefunction, whereas a single run of a quantum walk
experiment provides only one measurement outcome. Repetitions of the experiment thus need
to be quick and simple if a single result doesn’t provide a useful answer. This favours photonic
implementations over trapped atoms or ions.

Decohering quantum walks are more challenging for a classical computation, reducing the largest
classical simulation size to around $10^5$ sites. However, while classical simulations of this size can be
fully general without significant extra overhead, the experimental challenges may limit the types
of decoherent quantum walks that can be successfully created in the laboratory.

Although single quantum walker experiments will find it hard to beat classical computers, mul-
tiple interacting quantum walkers (quantum cellular automata) are a realistic goal for experiments
that reach beyond the scope of classical numerical simulation. They have a Hilbert space of size
$L^m$ for $m$ walkers on $L$ sites. For $L = 10$ sites, $m = 12$ walkers could outperform a classical
computer. The optimal architecture for this is atoms or ions in optical lattices, since the natural
interactions between the trapped atoms or ions are well-suited to the task. The immediate chal-
lenge is to identify quantum walk-based problems worth solving – in any architecture – that may
be experimentally accessible before general purpose quantum computers are built, and to design
the experiments that can implement them.

Acknowledgments

Thanks to Erika Andersson, Christine Silberhorn and Andrew White for useful discussions. Inspi-
ration for the title came from my friend Reb Gowers’ novel “When to Walk”. VK is funded by a
UK Royal Society University Research Fellowship.

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