Solid State Implementation of Quantum Random Walks on General Graphs

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Abstract. Advances in recent years have made it possible to explore quantum dots as a viable technology for scalable quantum information processing. Charge qubits for example can be realized in the lowest bound states of coupled quantum dots and the precision control of the confinement potential allows for the realization of a full set of universal qubit gates, including arbitrary single-qubit rotations and two-qubit C-NOT gates. In this work we describe a novel scheme for implementing quantum random walks on arbitrarily complex graphs by extending these elementary operations to the control of a two-dimensional quantum dot grid. As single-qubit rotations constitute the essential building blocks of our implementation scheme, we also present numerical simulations of one such mechanism by directly solving the corresponding time-dependent Schrödinger equation.

Keywords: Quantum random walk, quantum dynamics, charge qubits, quantum gates
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INTRODUCTION

The remarkable speed-up observed in the Shor factorization algorithm [1] and the Grover search algorithm [2] has prompt intense interest in developing appropriate physical systems for quantum computation and quantum information processing. Among the various proposals, solid-state systems are particularly attractive, since they are potentially ready to be integrated into large quantum networks and are enticing to the present semiconductor industry.

Quantum Dots [3] have in particular inspired many solid-state based proposals for quantum information processing and are routinely manufactured in numerous laboratories. When confining exactly one electron, pairs of coupled quantum dots can naturally form qubits, the building blocks for quantum circuits. Charge qubits for example can be formally defined as \(\alpha|L\rangle + \beta|R\rangle\) where \(\alpha\) and \(\beta\) represent the single electron amplitude to be present in the the lowest bound states of the left and right quantum dot respectively. There have been a number of proposals for performing quantum operations on solid state charge qubits [4, 5, 6, 7]. In particular references [8, 9] have demonstrated that a precision control of the confinement barrier potential allows for the realization of arbitrary single-qubit rotations.

In this paper we utilize these elementary qubit operations as the basis of a novel scheme for physically implementing quantum random walks on any arbitrary undirected graph. To do so we will first provide a theoretical platform for quantum random walks on graphs followed by a description of our proposed physical implementation scheme. Finally we provide the results of our numerical simulations for performing robust qubit rotations, which are fundamental for implementing of the walk.

QUANTUM WALK ON A GRAPH

Motivation

Random walks have been employed in virtually every science related discipline to model everyday phenomena such as the DNA synapsis [10], animals’ foraging strategies [11], diffusion and mobility in materials [12] and exchange rate forecast [13]. They have also found algorithmic applications, for example, in solving differential equations [14], quantum monte carlo for solving the many body Schrödinger equation [15], optimization [16], clustering and classification [17], fractal theory [18] or even estimating the relative sizes of Google, MSN and Yahoo search engines [19].

Whilst the so called classical random walks have been successfully utilized in such a diverse range of applications, quantum random walks are expected to provide us with a new paradigm for solving many practical problems more efficiently [20, 21]. In fact quantum walks have already inspired efficient algorithms with applications in connectivity and graph theory [22, 23], as well as quantum search and element distinctness [24, 25], due to their non-intuitive and markedly different properties, including faster mixing and hitting times.

To illustrate, take Alice, who is a classical random walker originally positioned at \(x = 0\). To decide whether to take a step to the left or right, he flips a coin with the two possible outcomes labeled by + and − and respec-
tive probabilities $P_+$ and $P_-$. Looking at the outcome, she then knows with certainty which way to move; either to the left ($x = -1$) or to the right ($x = +1$). Hence after many iterations of this process Alice’s classical walk traces a single path within a decision tree and the probability for finding him at a given position $x$ follows a Gaussian distribution. Meanwhile Bob, who is a quantum walker, flips his coin but never looks at the outcome. Instead he steps simultaneously to the left and right with complex amplitudes $\alpha_+$ and $\alpha_-$ such that $|\alpha_+|^2 = P_+$ and $|\alpha_-|^2 = P_-$. After many interactions Bob’s quantum walk results in a probability wavefunction with a finite amplitude to be present everywhere in the tree. At the end we can get Bob back in one piece by “collapsing” his wavefunction. This will allow him to emerge at some position $x$ with a probability given by the peculiar distribution depicted in Fig 1.

**Theory**

Let us first consider a complete graph with all possible connections between the $\mathcal{N}$ nodes including self loops. We will relax this constraint later by removing the unwanted connections. Here the walker requires an $\mathcal{N}$-sided coin for moving from one node to $\mathcal{N}$ other nodes. The complete state of the walker is therefore described by $|\psi\rangle = \sum_{j=1}^{\mathcal{N}} \sum_{k=1}^{\mathcal{N}} \alpha_{jk} |j, k\rangle$, where $|j\rangle$ denotes the nodes or position states of the walker, $|k\rangle$ specifies the state of the coin, and $\alpha_{jk}$ is a complex amplitude. A coin flip in the context of this quantum walk corresponds to a unitary rotation of the coin states at every node $j$ using an $\mathcal{N} \times \mathcal{N}$ matrix $\hat{c}_j$ also known as the coin operator. The coin operation is followed by the walker stepping from node $j$ simultaneously to all other nodes on the graph using a conditional translation operator $\hat{T}$ such that $\hat{T} |j, k\rangle \rightarrow |j', k\rangle$ according to some predefined rule, where $j$ and $j'$ label the two nodes at the end of an edge $e_{jj'}$ [39]. The quantum walk evolves via repeated applications of the coin followed by the translation operator. More explicitly

$$|\psi_n\rangle = \hat{T}_n \hat{c}_n \ldots \hat{T}_2 \hat{c}_2 \hat{T}_1 \hat{c}_1 |\psi_0\rangle,$$  

(1)

where $|\psi_0\rangle$ is the initial state of the walker, $|\psi_n\rangle$ corresponds to the state of the walk after $n$ steps, $\mathcal{N}^2 \times \mathcal{N}^2$ matrices $\hat{c}_i$ and $\hat{T}_i$ are the coin and translation operators at the $i$th step, and $\hat{c}_i$ incorporates the individual coin operators $\hat{c}_1 \ldots \hat{c}_N$ which simultaneously act on all the nodes. The operators $\hat{c}$ can in principle invoke different rotations at each node $j$, but are often uniformly set to be the Hadamard matrix.

In [38] we have shown that for any arbitrary graph the Hilbert space of the walk can in fact be represented as a two-dimensional $\mathcal{N} \times \mathcal{N}$ grid (Fig 2) where each individual node on the graph corresponds to a grid row (column) and the coin states within that node are the individual grid elements along that row (column). There, it is also shown that the quantum walk evolution given in Eq. 1 can effectively be reduced to

$$|\psi_n\rangle = \hat{c}_{nN}^\dagger \hat{c}_{nN-1}^\dagger \ldots \hat{c}_2^\dagger \hat{c}_1^\dagger |\psi_0\rangle,$$  

(2)
where $\hat{c}^H_i$ ($\hat{c}^V_j$) correspond to the application of the coin operator for the $i$th step, on the grid elements that are grouped horizontally (vertically) as depicted in Fig. 2.

Any general graph can now be constructed from its corresponding complete graph by removing the unwanted edges as depicted in Fig. 2. Eliminating an edge $e_{ij}$ corresponds to eliminating the connection between two states $|j, j\rangle$ and $|j, j\rangle$. However instead of removing these states from the Hilbert space, the action of the coin operators $\hat{c}^H_i$ ($\hat{c}^V_j$) can be altered in such a way as to isolate the unwanted states from interacting with other states.

![Figure 2](image.png)

**FIGURE 2.** a) A complete graph with $\mathcal{N} = 6$ nodes. b) The quantum walk Hilbert space viewed as a 2D array, where the element $(j, k)$ represents the state $k$ under node $j$. A generalized graph can be constructed by removing edges (dotted lines) from a complete graph. This can be physically achieved by modifying the coin operators in such a way as to isolate the unwanted states (dotted circles) from interacting with other states.

**PHYSICAL IMPLEMENTATION**

We propose utilizing a two-dimensional grid of quantum dots to represent the quantum walk’s Hilbert space, where the initial distribution of a single electron wave function among the dots represents the initial state of the walk. As we will see this scheme necessitates the construction of a $2 \times 2 \mathcal{N}$ grid, where every second row (column) of dots will be used as temporary “register”. In what follows we present a mechanism for manipulating the electronic wave function throughout the grid by introducing appropriate quantum dot interactions in a manner which corresponds exactly to the quantum random walk evolution described in Eq. 2. Naturally the resulting electron probability wave distribution gives the final state of the quantum walk.

Considering the evolution of the walk in Eq. 2, what we require is a means by which we can implement the action an arbitrary $\mathcal{N}$-level unitary operator $\hat{c}^H_i$ ($\hat{c}^V_j$) on the $\mathcal{N}$ nodes along the $j$th row (column) of the grid. In [38] we showed that this can be achieved via a CS decomposition [40] which essentially reduces a general $\mathcal{N}$-level rotation matrix to a series of pair-wise or qubit rotations which can in principle be readily implemented. What makes this implementation scheme non-trivial however is the fact that the resulting pair-wise interactions are not limited to neighboring nodes. More precisely it can be shown that for a general rotation of column $j$ for example, we have

$$\hat{c}^V_j = \prod_{d=1}^{\mathcal{N}-1} \hat{U}_d(d),$$

for $d \in \{2, 4, \ldots, \mathcal{N}/2\}$, where the action of each $\hat{U}_d(d)$ on the nodes of row $j$ consists of $\mathcal{N}/2$ simultaneous pair-wise interactions between nodes $kd + r$ and $kd + r + d/2$ where $k = 0, \ldots, \mathcal{N}/d - 1$, $d = 2, 4, \ldots, \mathcal{N}/2$ and $r = 1, 2, \ldots, d/2$. Clearly for all $\mathcal{N} \neq 2$, interactions are non-neighboring but follow a systematic form.

In the following sections we describe two mechanisms: 1) How to implement a pair-wise interaction between any two neighboring quantum dots, and 2) How to extend this to non-neighboring quantum dots.

**Pair-wise Interactions**

A pair of neighboring quantum dots can be made to undergo a unitary rotation $R$ by the precision control of the potential barrier between them [8, 9]. Assuming that the confined electron is initially in the left dot for example (Fig. 3), by dropping the barrier the electron wave packet is free to move between the two dots. Returning the barrier to its initial state at a precise moment in time makes it possible to recapture the electron but this time with the desired distribution across the two dots. We have presented a numerical simulation of this scheme in the last section.

Here we adopt the usual terminology to describe a $\pi$ rotation as one in which the electron wave-packet is
transferred entirely from one dot to its neighboring dot. This is also equivalent to a SWAP or NOT gate. Likewise a $\pi/2$ rotation represents a 50 – 50 split of the wave-packet initially confined to either of the dots.

![FIGURE 3](image)

Quantum Dot Conveyor Belt

To interact a pair of non-neighboring quantum dots we are effectively forced to move the two dots close to each other, apply the desired rotation and then return them to their original location.

What makes this process systematic and practically viable is the specific pattern of pairwise interactions arising from Eq. 3. As depicted in Fig. 4, to implement the action of each $U_i(d)$ we take the following five steps:

1. Apply $N/2$ simultaneous $\pi$ rotations to pairs of quantum dots at $kd + r$ and their adjacent register dot. This has the effect of transferring the electron wave packets to the register dots.

2. Adiabatically move the register quantum dots, much like a "conveyor belt" carrying the electron wavepackets along the register row (column). This can be archived by carefully designing and manipulating the voltage applied to the electrodes such that the confinement potentials experience an effective motion. Moving the register dots by an amount equal to $d$ times the quantum dot width would effectively allow the amplitudes at $kd + r$ to be coupled with the amplitudes at $kd + r + d/2$.

3. Simultaneously apply $N/2$ general rotations $\hat{R}$ to the newly coupled quantum dot pairs.

4. Return the register qubits to their original location by reversing the adiabatic motion;

5. Introduce another $\pi$ rotation to move the amplitudes from register dots back to their original positions.

We emphasis that the above steps can be carried out simultaneously throughout the entire grid and the rotation $\hat{R}$ in step 3 can be different for each quantum dot pair.

![FIGURE 4](image)

Modeling Qubit Rotations

One of the key issues in quantum computation is to design a time-dependent Hamiltonian as precisely as possible, so that one can drive the system undergo the required logic gate manipulation. Since the intrinsic parallelism of a quantum computer comes from superposition and entanglement where phases and amplitudes play an eminently important role, such a design can only be achieved through detailed theoretical calculations including all perceptible interactions in the system.

The Schrödinger equation governing the quantum dynamical evolution of few-electron systems reads

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left[ \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m^*} \nabla_{r_i}^2 + V(\vec{r}_i) \right) + \frac{e^2}{4\pi\varepsilon} \sum_{i>j=1}^{N} \frac{1}{r_{ij}} \right] \psi(\vec{r}, t)$$
The above equation can be solved efficiently using a Chebychev polynomial expansion [41, 8]

\[
\psi(\vec{r}, t) = \exp(-i(E_{\text{max}} + E_{\text{min}})t/2) \sum J_n(\alpha) T_n(-i\tilde{H})\psi(\vec{r}, 0),
\]

where \( E_{\text{max}} \) and \( E_{\text{min}} \) are the upper and lower bounds on the energies sampled by the numerical grid, \( J_n(\alpha) \) are Bessel functions of the first kind, \( T_n \) are the Chebychev polynomials. The normalized Hamiltonian is defined as \( \tilde{H} = (2H - E_{\text{max}} - E_{\text{min}})/(E_{\text{max}} - E_{\text{min}}) \) to ensure convergence.

Using such a theoretical framework, all electrons in the system are treated on equal footing, and they evolve coherently in time under the influence of each other as well as external fields. Fig. 5 illustrates the time evolution of an electron confined in a coupled quantum dot system provided by the above equation. All possible qubit rotations in the Bloch sphere can be accomplished by controlling the central potential barrier and/or electron-electron interactions, as demonstrated in Fig. 6 where the amplitudes of and the phase between the \(|L\rangle\) and \(|R\rangle\) states are shown as time varies.

**FIGURE 5.** Time evolution of system wave-function in coupled quantum dot system.

**FIGURE 6.** Qubit rotation in the Bloch sphere as time varies.

**CONCLUSION**

In this paper, we provided a practical recipe for efficiently implementing quantum random walks on arbitrarily complex graphs using electrons trapped in a 2D array of quantum dots. The proposed scheme is particularly elegant since the walker is not required to physically step between the vertices of the associated graph, giving rise to a significant advantage over other existing schemes. Also presented is a detailed simulation of controlled qubit rotation in the Bloch sphere. Our numerical results show that even the simplest gate operations induce rather intricate quantum dynamics. Nonetheless, with precision control of the electrodes that define the coupled quantum dots, arbitrary qubit rotations in the Bloch sphere can be accomplished.

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