An example of the difference between quantum and classical random walks

Andrew M. Childs,[1] Edward Farhi,[1] and Sam Gutmann[2]
[1] *Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139*
[2] *Department of Mathematics, Northeastern University, Boston, MA 02115*
(5 March 2001)

In this note, we discuss a general definition of quantum random walks on graphs and illustrate with a simple graph the possibility of very different behavior between a classical random walk and its quantum analogue. In this graph, propagation between a particular pair of nodes is exponentially faster in the quantum case. [MIT-CTP #3093]

Introduction. Many classical algorithms are based on random walks, so it is natural to ask whether quantum random walks might be useful for quantum computation. A framework for using quantum random walks to solve decision problems was investigated in [1]. There also, an exponential separation was found between the classical and quantum times to propagate through a certain tree.

In this note, we describe a general definition of continuous-time random walks on graphs and give a simpler example of a graph for which the quantum time to propagate between a particular pair of nodes is exponentially shorter than the analogous classical propagation time. We also discuss advantages of the continuous time formulation over discrete versions.

Random walks. A continuous time classical random walk on a graph is a Markov process. A graph is a set of v vertices $\{1, 2, \ldots, v\}$ and a set of edges that specifies which pairs of vertices are connected in the graph. A step in a classical random walk on a graph only occurs between two vertices connected by an edge. Let γ denote the jumping rate. Starting at any vertex, the probability of jumping to any connected vertex in a time ϵ is $\gamma\epsilon$ (in the limit $\epsilon \to 0$). This random walk can be described by the $v \times v$ infinitesimal generator matrix M defined by

$$M_{ab} = \begin{cases} -\gamma & a \neq b,\ a \text{ and } b \text{ connected by an edge} \\ 0 & a \neq b,\ a \text{ and } b \text{ not connected} \\ k\gamma & a = b,\ k \text{ is the valence of vertex } a. \end{cases} \quad (1)$$

If $p_a(t)$ denotes the probability of being at vertex a at time t, then

$$\frac{\mathrm{d}p_a(t)}{\mathrm{d}t} = -\sum_b M_{ab}\, p_b(t)\,. \quad (2)$$

Consider quantum evolution in a v-dimensional Hilbert space according to a Hamiltonian H. In a basis $|1\rangle, |2\rangle, \ldots, |v\rangle$, the Schrödinger equation for $|\psi(t)\rangle$ can be written

$$i\frac{\mathrm{d}}{\mathrm{d}t}\langle a|\psi(t)\rangle = \sum_b \langle a|H|b\rangle\langle b|\psi(t)\rangle\,. \quad (3)$$

Note the similarity between (2) and (3). Whereas (2) conserves probability in the sense that

$$\sum_a p_a(t) = 1\,, \quad (4)$$

the Schrödinger equation preserves probability as the sum of the amplitudes squared:

$$\sum_a |\langle a|\psi(t)\rangle|^2 = 1\,. \quad (5)$$

In some sense, *any* evolution in a finite-dimensional Hilbert space can be thought of as a "quantum random walk." However, the analogy is clearest when H has an obvious local structure.

A quantum random walk on a graph is naturally defined in a Hilbert space spanned by basis elements corresponding to the vertices. To respect the structure of the graph, we require that for $a \neq b$,

$$\langle a|H|b\rangle \neq 0 \text{ iff } a \text{ and } b \text{ are connected by an edge.} \quad (6)$$

This is a very weak requirement, so we can impose more structure on H. A natural quantum analogue to the classical random walk described above is given by the quantum Hamiltonian with matrix elements [1]

$$\langle a|H|b\rangle = M_{ab}\,. \quad (7)$$

Note that on a one-dimensional lattice, this results in the Hamiltonian defined by

$$H|j\rangle = -\frac{1}{\Delta^2}(|j-1\rangle - 2|j\rangle + |j+1\rangle)\,, \quad (8)$$

which is just a discrete approximation to the operator $-\mathrm{d}^2/\mathrm{d}x^2$ (where $\Delta = \gamma^{-1/2}$ is the lattice spacing).

The difference between the quantum and classical evolution comes from the i which appears in (3) but not in (2). This can result in radically different behavior, as seen in [1]. A simpler example is given next.

An example. Here we define a sequence of graphs G_n. The number of vertices in G_n is $2^{n+1}+2^n-2$. In Figure 1 we show G_4. In general, G_n consists of two balanced binary trees of depth n with the 2^n nth-level vertices of the two trees pairwise identified.

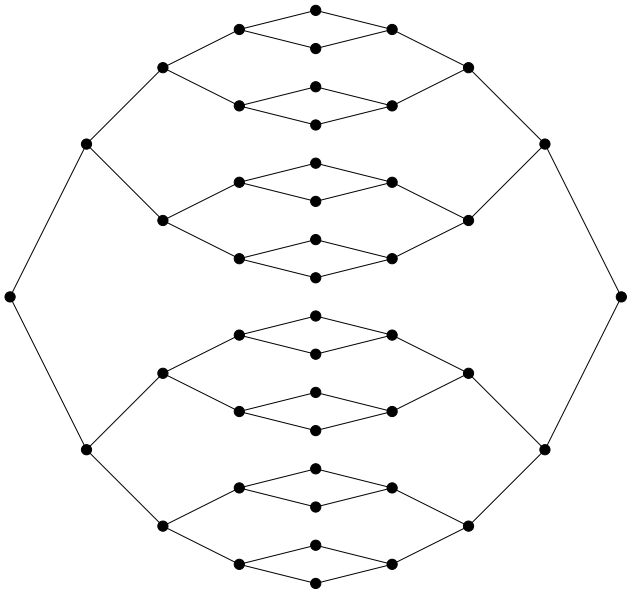

FIG. 1. The graph G_4.

For both the classical and quantum random walks, we start at the root of one tree and want the probability as a function of time of being at the other root. In other words, we are interested in how long it takes to propagate from the leftmost vertex to the rightmost vertex as a function of n.

Consider the classical case first. The vertices of G_n can be grouped in columns indexed by $j \in \{0, 1, \ldots, 2n\}$. Column 0 contains the root of the left tree, column 1 contains the two vertices connected to that root, etc. Note that column n contains the 2^n vertices in the middle of the graph and column $2n$ is the root at the right.

To analyze the classical walk from the left root to the right root, we need only keep track of the probabilities of being in the columns. In the left tree, for $0 < j < n$, the probability of stepping from column j to column $j+1$ is twice as great as the probability of stepping from column j to column $j-1$. However, in the right tree, for $n < j < 2n$, the probability of stepping from column j to column $j+1$ is half as great as the probability of stepping from column j to column $j-1$. This means that if you start at the left root, you quickly move to the middle of the graph, but then it takes a time exponential in n to reach your destination. More precisely, starting in column 0, the probability of being in column $2n$ after any number of steps is less than 2^{-n}. This implies that the probability of reaching column $2n$ in a time that is polynomial in n must be exponentially small as a function of n.

We now analyze the quantum walk on G_n starting in the state corresponding to the left root and evolving with the Hamiltonian given by (7). With this initial state, the symmetries of H keep the evolution in a $(2n+1)$-dimensional subspace of the $(2^{n+1}+2^n-2)$-dimensional Hilbert space. This subspace is spanned by states $|\text{col } j\rangle$ (where $0 \le j \le 2n$), the uniform superposition over all vertices in column j, that is,

$$|\text{col } j\rangle = \frac{1}{\sqrt{N_j}} \sum_{a \in \text{column } j} |a\rangle\,, \tag{9}$$

where

$$N_j = \begin{cases} 2^j & 0 \le j \le n \\ 2^{2n-j} & n \le j \le 2n\,. \end{cases} \tag{10}$$

In this basis, the non-zero matrix elements of H are

$$\langle \text{col } j|H|\text{col } j \pm 1\rangle = -\sqrt{2}\gamma \tag{11}$$

$$\langle \text{col } j|H|\text{col } j\rangle = \begin{cases} 2\gamma & j = 0, n, 2n \\ 3\gamma & \text{otherwise,} \end{cases} \tag{12}$$

which is depicted in Figure 2 (for $n = 4$) as a quantum random walk on a line with $2n+1$ vertices.

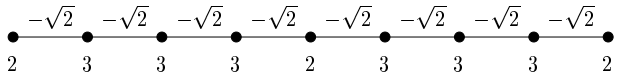

FIG. 2. The reduction of G_4 to a quantum random walk on a line. Vertices correspond to columns and are labeled with the diagonal matrix elements of H/γ, whereas edges are labeled with its matrix elements between adjacent columns.

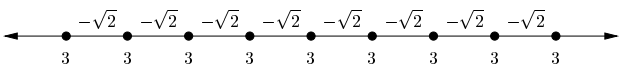

FIG. 3. Quantum random walk on an infinite, translationally invariant line.

Starting at the leftmost vertex of Figure 2, there is an appreciable probability of being at the rightmost vertex after a time proportional to n. To see this, first consider quantum propagation on an infinite, translationally invariant line of vertices as depicted in Figure 3. Here it is straightforward to compute the amplitude to go from vertex l to vertex m in a time t (for example, see [2]):

$$\langle m|e^{-iHt}|l\rangle = e^{-i3\gamma t} i^{m-l} J_{m-l}(2\sqrt{2}\gamma t)\,, \tag{13}$$

where J_{m-l} is a Bessel function of order $m-l$. This corresponds to propagation with speed $2\sqrt{2}\gamma$. More precisely, for any $\epsilon > 0$ and $|m-l| \gg 1$, for $t < \left(\frac{1}{2\sqrt{2}\gamma} - \epsilon\right)|m-l|$, the amplitude is exponentially small in $|m-l|$, whereas there are values of t between $(\frac{1}{2\sqrt{2}\gamma})|m-l|$ and $(\frac{1}{2\sqrt{2}\gamma} + \epsilon)|m-l|$ at which the amplitude is of order $|m-l|^{-1/2}$.

In the limit of large n, the reduced version of G_n is nearly identical to the infinite, translationally invariant line, so it is plausible that propagation on G_n will also occur with speed $2\sqrt{2}\gamma$. To verify this, we numerically compute the probability $|\langle \text{col } j|\psi(t)\rangle|^2$ of being in column j at various times t, where $|\psi(0)\rangle = |\text{col } 0\rangle$ and we choose $\gamma = 1$. This is shown in Figure 4 with $n = 500$ for

$t = 100$, 250, and 400. These plots clearly show a wave packet which propagates with speed $2\sqrt{2}$, with the amplitude near the wavefront decreasing like $t^{-1/2}$. In the first plot, at $t = 100$, the leading edge of the distribution is at column $200\sqrt{2} \approx 283$. The packet has not yet encountered the small defect at the center, so it has a relatively simple shape. At $t = 250$, the wavefront has passed the center, and a small reflection can be seen propagating backward. However, the leading edge is relatively undisturbed, having propagated to column $500\sqrt{2} \approx 707$. The wavefront continues to propagate with speed $2\sqrt{2}$ until it reaches the right root, where the packet is reflected. The last plot, at $t = 400$, shows the distribution shortly after this first reflection. Even after the reflection, there is still an appreciable probability of being at the right root.

The limiting distribution. In this section, we consider the distribution over the vertices after a long time. We emphasize that although the mixing times (the characteristic times to reach the limiting distribution) may be similar in the classical and quantum cases [3], this is in no way indicative of similar dynamics, as the limiting distributions may be radically different.

In the classical case, the limiting distribution is defined as

$$\pi_b = \lim_{T\to\infty} p_b(T)\,, \tag{14}$$

which is independent of the starting state. It is easy to see that the limiting distribution on G_n is uniform over the vertices: this distribution is the unique eigenvector of M with eigenvalue 0, so it is the only component that remains after a long time. Thus $\pi_b = (2^{n+1} + 2^n - 2)^{-1}$ for each vertex b, which is exponentially small.

In the quantum case, unitarity prevents the walk from reaching a steady state. However, a sensible definition of the limiting distribution, which depends on the initial state $|a\rangle$, is given by [3]

$$\chi_b = \lim_{T\to\infty} \frac{1}{T} \int_0^T |\langle b|e^{-iHt}|a\rangle|^2 \,\mathrm{d}t\,. \tag{15}$$

This is the distribution resulting from a measurement done after a time chosen uniformly in $[0, T]$, in the limit of large T. By expanding over the energy eigenstates $|E_r\rangle$, we find

$$\chi_b = \sum_{r,s} \langle b|E_r\rangle\langle E_r|a\rangle\langle a|E_s\rangle\langle E_s|b\rangle \times \lim_{T\to\infty} \frac{1}{T} \int_0^T e^{-i(E_r - E_s)t}\,\mathrm{d}t \tag{16}$$

$$= \sum_r |\langle a|E_r\rangle|^2\, |\langle b|E_r\rangle|^2 \tag{17}$$

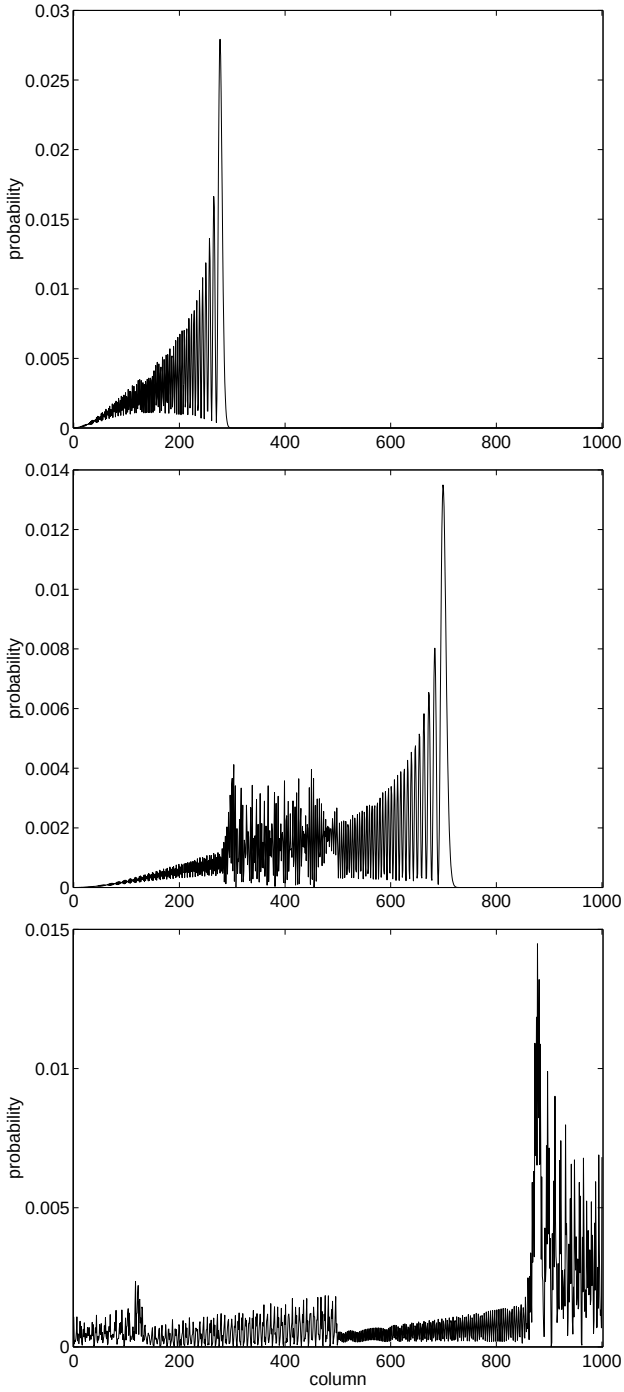

FIG. 4. Propagation in G_{500} starting at the left root. From top to bottom, the times are $t = 100$, 250, and 400.

(note that we have assumed $E_r \neq E_s$ for $r \neq s$, which is true for G_n). In particular, consider the case where $|a\rangle = |\mathrm{col}\ 0\rangle$ corresponds to the left root and $|b\rangle = |\mathrm{col}\ 2n\rangle$ corresponds to the right root. In this case, we may work in the reduced Hilbert space spanned by the columns, so the number of energy eigenstates is $2n + 1$. By symmetry, $|\langle \mathrm{col}\ 0|E_r\rangle| = |\langle \mathrm{col}\ 2n|E_r\rangle|$. The Cauchy-Schwartz inequality gives

$$\sum_r |\langle \text{col } 0|E_r\rangle|^4 \sum_s 1 \geq \left(\sum_r |\langle \text{col } 0|E_r\rangle|^2 \right)^2 = 1\,, \quad (18)$$

which implies

$$\sum_r |\langle \text{col } 0|E_r\rangle|^4 \geq \frac{1}{2n+1}\,. \quad (19)$$

Thus in the limiting distribution, the probability of being at the right root, starting at the left root, is

$$\chi_{\text{col } 2n} \geq \frac{1}{2n+1}\,, \quad (20)$$

which is much larger than in the classical case.

Discussion. The model of quantum random walks used in this note applies automatically to any graph. In particular, the Hamiltonian is determined by the local structure of the graph and its definition does not require knowledge of any global properties. It is easy to imagine situations where the local structure of a graph is readily accessible, but determining some global property is difficult. For example, a computational problem may involve searching a graph for a node with a certain property whose presence or absence from the graph corresponds to the solution of an NP-complete problem [1].

The Hamiltonian-based approach to quantum random walks can be contrasted with discrete time models (for example, see [3–5]) involving the extra state space of a "quantum coin." This extra label seems to be necessary in discrete time formulations of quantum random walks (and is provably necessary in the one dimensional case [6]). However, for general graphs of mixed valence, it is not obvious how to define the discrete time unitary evolution operator without knowledge of global properties of the graph.

Acknowledgements. This work was supported in part by the Department of Energy under cooperative agreement DE-FC02-94ER40818. AMC is supported by the Fannie and John Hertz Foundation.

[1] E. Farhi and S. Gutmann, *Quantum computation and decision trees*, Phys. Rev. A **58**, 915 (1998).

[2] E. Farhi and S. Gutmann, *The functional integral constructed directly from the Hamiltonian*, Ann. Phys. **213**, 182 (1992).

[3] D. Aharonov, A. Ambainis, J. Kempe, and U. Vazirani, *Quantum walks on graphs*, quant-ph/0012090.

[4] Y. Aharonov, L. Davidovich, and N. Zagury, *Quantum random walks*, Phys. Rev. A **48**, 1687 (1993).

[5] A. Nayak and A. Vishwanath, *Quantum walk on the line*, quant-ph/0010117.

[6] D. A. Meyer, *From quantum cellular automata to quantum lattice gasses*, J. Stat. Phys. **85**, 551 (1996).