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ON MIXING IN CONTINUOUS-TIME QUANTUM WALKS ON SOME CIRCULANT GRAPHS

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Classical random walks on well-behaved graphs are rapidly mixing towards the uniform distribution. Moore and Russell showed that the continuous-time quantum walk on the hypercube is instantaneously uniform mixing. We show that the continuous-time quantum walks on other well-behaved graphs do not exhibit this uniform mixing. We prove that the only graphs amongst balanced complete multipartite graphs that have the instantaneous exactly uniform mixing property are the complete graphs on two, three and four vertices, and the cycle graph on four vertices. Our proof exploits the circulant structure of these graphs. Furthermore, we conjecture that most complete cycles and Cayley graphs of the symmetric group lack this mixing property as well.

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1. Introduction

Two pervasive algorithmic ideas in quantum computation are Quantum Fourier Transform (QFT) and amplitude amplification (see [2]). Most subsequent progress in quantum computing owed much to these two beautiful ideas. But there are many problems whose characteristics matches neither the QFT nor the amplitude amplification mold (e.g., the Graph Isomorphism problem). This begs for new additional tools to be discovered.

A natural way to discover new quantum algorithmic ideas is to adapt a classical one to the quantum model. An appealing well-studied classical idea in statistics and computer science is the method of random walks [3, 4]. Recently, the quantum analogue of classical random walks has been studied in a flurry of works [5, 6, 7, 8, 9, 10]. The works of Moore and Russell [9] and Kempe [10] showed faster bounds on instantaneous mixing and hitting times for discrete and continuous-time quantum walks on the hypercube (compared to the classical walk).

The focus of this note is on the *continuous-time* quantum walk that was introduced by Farhi and Gutmann [5]. In a subsequent paper, Childs et al. [6] gave a simple example where the classical and (continuous-time) quantum walks exhibit a different behavior in hitting time statistics. The goal of this note is to show further qualitative differences (by elementary means) between the two models in their mixing time behaviors. A main result is that, on the natural class of complete and balanced complete multipartite graphs, only the complete graphs K_n on $n = 2, 3, 4$ vertices and the cycle graph of size four (i.e., $K_{2,2}$) have the instantaneous exactly uniform mixing property, i.e., there exists a time when the probability distribution function of the quantum walk is exactly the uniform distribution. This is distinctly different from the classical walk and from the discrete quantum walk. The proofs of these exploit heavily the circulant structure of these graphs.

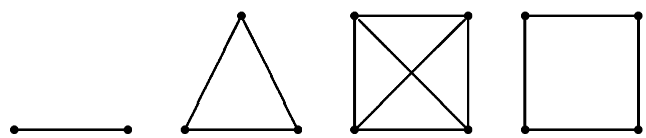

Fig. 1. The only balanced multipartite graphs with the continuous-time instantaneous uniform mixing property. From left to right: K_2, $K_3 = C_3$, K_4, and $K_{2,2} = C_4$.

A recent work by Childs et al. [1] gave an interesting and powerful algorithmic application of continuous-time quantum walks.

Thus far, there are two relevant notions of *mixing* in quantum walks: *instantaneous* and *average*. To our knowledge, Moore and Russell [9] were the first to introduce and study *instantaneous* mixing, in contrast to the notion of *average* mixing defined by Aharonov et al. [8]. Moore and Russell [9] proved that the hypercubes have the instantaneous exactly uniform property. They also observed that in the case of hypercubes (or large connected graphs), the notion of instantaneous mixing time is more relevant than the notion of average mixing time, since the quantum walk is never close to uniform in the average sense and is close to uniform only for small time intervals. Their observations suggest looking at the instantaneous mixing of continuous-time quantum walks on large connected graphs, such as complete graphs and complete bipartite graphs, which is the topic of this work.

To the best of our knowledge, the algorithmic application of mixing in quantum walk has yet to be explored. Classical applications of rapid mixing of random walks, such as counting and random generation of combinatorial structures, might be natural settings for future investigations.

2. Continuous-time quantum walks

Continuous-time quantum walks was introduced by Farhi and Gutmann [5] (see also [6, 9]). Our treatment, though, follow closely the analysis of Moore and Russell [9], which we review next. Let $G = (V, E)$ be a simple, undirected, connected, d-regular n-vertex graph. Let A be the adjacency matrix of G defined as

$$A_{jk} = \begin{cases} 1 & \text{if } (j,k) \in E \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

We consider the transition matrix $H = \frac{1}{d}A$ (treated as the Hamiltonian of the quantum system). Let the initial amplitude wave function of the particle be $|\psi_0\rangle = |0\rangle$. Then, the amplitude wave function at time t, is given by Schrödinger's equation, as

$$i\hbar\frac{\mathsf{d}}{\mathsf{d}t}|\psi_t\rangle = H|\psi_t\rangle. \tag{2}$$

or (assuming from now on $\hbar = 1$) $|\psi_t\rangle = e^{-iHt}|\psi_0\rangle$. This is similar to the model of a continuous-time Markov chain in the classical sense (see [11]). It is more natural to deal with the Laplacian of the graph, defined as $L = A - D$, where D is a diagonal matrix with entries $D_{jj} = deg(v_j)$. This is because we can view L as the generator matrix that describes an exponential distribution of waiting times at each vertex. But on d-regular graphs, $D = \frac{1}{d}I$, and since A and D commute, we get $e^{-itL} = e^{-it(A-\frac{1}{d}I)} = e^{-it/d}e^{-itA}$; this introduces an irrelevant phase factor in the wave evolution.

The probability that the particle is at vertex j at time t is given by

$$P_t(j) = |\langle j|\psi_t\rangle|^2. \tag{3}$$

The *average* probability that the particle is at vertex j is given by

$$P(j) = \lim_{T\to\infty}\frac{1}{T}\int_0^T P_t(j)\mathsf{d}t. \tag{4}$$

Since H is Hermitian, the matrix $U_t = e^{-iHt}$ is unitary. If $(\lambda_j, |z_j\rangle)_j$ are the eigenvalue and eigenvector pairs of H, then $(e^{-i\lambda_j t}, |z_j\rangle)_j$ are the eigenvalue and eigenvector pairs of U_t. Because H is symmetric, there is an orthonormal set of eigenvectors, say $\{|z_j\rangle : j \in [n]\}$ (i.e., H is unitarily diagonalizable). So, if $|\psi_0\rangle = \sum_j \alpha_j|z_j\rangle$, then

$$|\psi_t\rangle = \sum_j \alpha_j e^{-i\lambda_j t}|z_j\rangle. \tag{5}$$

Definition 1 *(instantaneous and average mixing [9, 8])*
Let $\epsilon \geq 0$. A graph $G = (V,E)$ has the instantaneous *ϵ-uniform* mixing *property if there exists $t \in \mathbb{R}^+$, such that the continuous-time quantum walk on G satisfies $||P_t - U|| \leq \epsilon$, where $||Q_1 - Q_2|| = \sum_x |Q_1(x) - Q_2(x)|$ is the total variation distance between two probability distributions Q_1, Q_2, and U is the uniform distribution on the vertices of G. Whenever $\epsilon = 0$ is achievable, G is said to have instantaneous exactly uniform mixing.*

The graph $G = (V,E)$ has the average *uniform* mixing *property if the average probability distribution satisfies $P(j) = 1/|V|$, for all $j \in V$.*

A random walk on G is called *simple* if the transition probability matrix is $H = \frac{1}{d}A$, where A is the adjacency matrix of the d-regular graph G. The walk is called *lazy* if, at each step, the walk stays at the current vertex with probability $\frac{1}{2}$ and moves according to H with probability $\frac{1}{2}$. For continuous-time quantum walks, these two notions are *equivalent* modulo a time scaling. Again, the argument is by exploiting the commutativity of A and I (that introduces an irrelevant phase factor in the amplitude expression).

3. A simple example

This section describes an example, on the complete graph K_2 with two vertices, illustrating the differences between classical (discrete and continuous-time) random walk and continuous-time quantum walk. The adjacency matrix of K_2 is $A = X$, the Pauli X matrix. Since K_2 is bipartite, a simple random walk starting at any vertex will oscillate between the two states; hence never reaches the uniform distribution. However, the *lazy* random walk, with transition matrix $\frac{1}{2}(I + A)$, converges to the uniform distribution after a single step.

Let us consider a continuous-time walk with generator matrix $Q = \begin{pmatrix} -\alpha & \beta \\ \alpha & -\beta \end{pmatrix}$. This is viewed as a two-state chain where a transition is made after exponentially distributed waiting times with rates α and β from states 1 and 2, respectively (see [11], page 156). Note that Q has eigenvalues $0, -(\alpha+\beta)$ with the respective eigenvectors of $(\beta \quad \alpha)^T$, $(1 \quad -1)^T$. Let $P(t)$ be the matrix with entries $p_{jk}(t) = \Pr(X(t) = k \mid X(0) = j)$ describing the evolution of the continuous-time walk after t steps. It is known that

$$\frac{\mathsf{d}}{\mathsf{d}t}P(t) = QP(t), \tag{6}$$

which implies $P(t) = e^{tQ}$. Note that Q can be diagonalized using the matrices

$$B = \begin{pmatrix} 1 & \beta \\ -1 & \alpha \end{pmatrix}, \quad B^{-1} = \frac{1}{\alpha+\beta}\begin{pmatrix} \alpha & -\beta \\ 1 & 1 \end{pmatrix}. \tag{7}$$

Therefore,

$$P_t = e^{tQ} = B\begin{pmatrix} e^{-t(\alpha+\beta)} & 0 \\ 0 & 1 \end{pmatrix}B^{-1} = \frac{1}{\alpha+\beta}\begin{pmatrix} \alpha e^{-t(\alpha+\beta)} + \beta & \beta(1-e^{-t(\alpha+\beta)}) \\ \alpha(1-e^{-t(\alpha+\beta)}) & \beta e^{-t(\alpha+\beta)} + \alpha \end{pmatrix}. \tag{8}$$

So, the uniform distribution is reached in the limit if and only if $\alpha = \beta = 1$.

Finally, we consider the continuous-time quantum walk, where the wave amplitude vector at time t is

$$|\psi_t\rangle = e^{-itA}|0\rangle = \begin{pmatrix} \cos(t) \\ -i\sin(t) \end{pmatrix} \implies P_t = \begin{pmatrix} \cos^2(t) \\ \sin^2(t) \end{pmatrix}. \tag{9}$$

The latter reaches the uniform distribution periodically at $t = k\pi + \pi/4$, for $k \in \mathbb{Z}^+$. So, the continuous-time quantum walk on K_2 has the instantaneous exactly uniform mixing property. The average probabilities are $P(0) = P(1) = 1/2$, which is uniform, since $\lim_{T\to\infty} 1/T\int_0^T \cos^2(t)\mathsf{d}t = \lim_{T\to\infty} 1/T\int_0^T \sin^2(t)\mathsf{d}t = 1/2$. We will revisit this analysis under more general conditions in a subsequent section.

4. Circulant Graphs

A matrix A is circulant if its k-th row is obtained from the 0-th row by k consecutive right-rotations. A graph G is circulant if its adjacency matrix is a circulant matrix. Some examples of circulant graphs include complete graphs and complete cycles. An important property of circulant matrices is that they are (unitarily) diagonalizable by the Fourier matrix

$$F = \frac{1}{\sqrt{n}} V(\omega), \tag{10}$$

where $\omega = e^{2\pi i/n}$ and $V(\omega)$ is the Vandermonde matrix defined as

$$V(\omega) = \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \dots & \omega^{n-1} \\ 1 & \omega^2 & \omega^4 & \dots & \omega^{2(n-1)} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & \omega^{n-1} & \omega^{2(n-1)} & \dots & \omega^{(n-1)^2} \end{pmatrix}. \tag{11}$$

Let the j-th column vector of $V(\omega)$ be denoted by $|\omega_j\rangle$, $j = 0, \dots, n-1$. It is easy to verify that F is unitary, i.e., $F^{-1} = F^\dagger$, since the Vandermonde matrix obeys $V(\omega)^{-1} = V(\omega^{-1})$. If C is a circulant matrix whose 0-th column vector is $|f\rangle$ then

$$FCF^\dagger = diag(V(\omega)|f\rangle). \tag{12}$$

5. The complete graph K_n

The adjacency matrix of K_n is $A = J_n - I_n$, where J_n is the all-one $n \times n$ matrix and I_n is the $n \times n$ identity matrix. The eigenvalues of $\frac{1}{n-1}A$ are 1 (once) and $-\frac{1}{n-1}$ ($n-1$ times). Using the orthonormal eigenvectors $|F_j\rangle \doteq \frac{1}{\sqrt{n}}|\omega_j\rangle$ (the columns of the Fourier matrix F), the initial amplitude vector is $|\psi_0\rangle = \frac{1}{n}\sum_j |\omega_j\rangle$. For $|\psi_t\rangle$, we have

$$\langle j|\psi_t\rangle = \begin{cases} -\frac{2}{n} e^{\frac{-it(n-2)}{2(n-1)}} sin\left(\frac{tn}{2(n-1)}\right) & \text{if } j \neq 0 \\ \frac{1}{n}(e^{-it} + (n-1)e^{it/(n-1)}) & \text{if } j = 0 \end{cases} \tag{13}$$

Thus

$$P_t(j) = \begin{cases} \frac{4}{n^2} sin^2\left(\frac{tn}{2(n-1)}\right) & \text{if } j \neq 0 \\ 1 - \frac{4(n-1)}{n^2} sin^2\left(\frac{tn}{2(n-1)}\right) & \text{if } j = 0 \end{cases} \tag{14}$$

Notice that to achieve exact uniformity, for all $j \neq 0$, we need $P_t(0) = P_t(j)$, or

$$\frac{4}{n} sin^2\left(\frac{tn}{2(n-1)}\right) = 1. \tag{15}$$

Thus, exact uniformity is possible only if $n = 2, 3, 4$. In contrast, a classical walk never achieves uniform on K_2, but converges to uniform on K_n, for all $n > 2$. Using elementary calculus, we also obtain the average probabilities:

$$P(j) = \begin{cases} \frac{2}{n^2} & \text{if } j \neq 0 \\ 1 - \frac{2(n-1)}{n^2} & \text{if } j = 0 \end{cases} \tag{16}$$

These observations are summarized in the following theorem.

Theorem 1 *No complete graph, except for K_2, K_3, and K_4, has the instantaneous exactly uniform mixing property under the continuous-time quantum walk model. Furthermore, no complete graph, except for K_2, has the* average *uniform mixing property under the continuous-time quantum walk model.*

Using the above bounds on $P_t(j)$, we calculate the total variation distance between P_t and the uniform distribution on $V(G)$. We obtain

$$||P_t - U|| = \sum_j |P_t(j) - 1/n| = 2(1 - 1/n)\left|1 - \frac{4}{n}\sin^2\left(\frac{tn}{2(n-1)}\right)\right|. \tag{17}$$

For large n, this suggests that P_t is never close to U. Similarly, the total variation distance between the average limiting probability P and U is given by $||P - U|| = (1-1/n)(1-2/n) + |1 - (3-2/n)/n|$. Again, this suggests that P is never close to U.

6. The balanced complete multipartite graphs

Let G be a complete a-partite graph where each partition has $b > 1$ vertices (the case $b = 1$ is the complete graph case). Let A be the normalized adjacency matrix of G. Note that A is given by

$$A = \frac{1}{a-1}K_a \otimes \frac{1}{b}J_b. \tag{18}$$

Using the circulant structure of both matrices, it is clear that the normalized eigenvalues of K_a are 1 (once) and $-\frac{1}{a-1}$ (with multiplicity $a-1$) and that the normalized eigenvalues of J_b are 1 (once) and 0 (with multiplicity $b-1$). Let $\alpha = e^{\frac{2\pi i}{a}}$ be the principal a-th root of unity and let $\beta = e^{\frac{2\pi i}{b}}$ be the principal b-th root of unity. Both matrices have the columns of the Fourier matrix of dimensions a and b, respectively, as their orthonormal set of eigenvectors. So let $\{|\alpha_j\rangle\}_{j=0}^{a-1}$ and $\{|\beta_k\rangle\}_{k=0}^{b-1}$ be the orthogonal sets of eigenvectors of K_a and J_b, respectively. Note that $|\alpha_0\rangle = |1_a\rangle$ and $|\beta_0\rangle = |1_b\rangle$.

The eigenvalues of A is $\lambda_0 = 1$ (once) with the all-one eigenvector $|1_a\rangle \otimes |1_b\rangle$, $\lambda_1 = -\frac{1}{a-1}$ (with multiplicity $a-1$) with the eigenvectors $|\alpha_j\rangle \otimes |1_b\rangle$, for $j = 1, 2, \ldots, a-1$. and $\lambda_2 = 0$ (with multiplicity $a(b-1)$) with eigenvectors $|\alpha_j\rangle \otimes |\beta_k\rangle$, for $1 \leq j < a$ and $1 \leq k < b$. Thus, the wave amplitude function $|\psi_t\rangle$ is

$$|\psi_t\rangle = \frac{1}{ab}\left[e^{-it}|1_a\rangle \otimes |1_b\rangle + e^{\frac{it}{a-1}}\sum_{j=1}^{a-1}|\alpha_j\rangle \otimes |1_b\rangle + \sum_{k=1}^{b-1}\sum_{j=1}^{a-1}|\alpha_j\rangle \otimes |\beta_k\rangle\right], \tag{19}$$

which equals to

$$|\psi_t\rangle = \frac{1}{ab}\left[e^{-it}\begin{pmatrix}|1_b\rangle \\ |1_b\rangle \\ \vdots \\ |1_b\rangle\end{pmatrix} + e^{\frac{it}{a-1}}\begin{pmatrix}|a\rangle - |1_b\rangle \\ -|1_b\rangle \\ \vdots \\ -|1_b\rangle\end{pmatrix} + \begin{pmatrix}a\sum_{k=1}^{b-1}|\beta_k\rangle \\ |0_b\rangle \\ \vdots \\ |0_b\rangle\end{pmatrix}\right]. \tag{20}$$

Thus, the wave amplitude expressions are

$$\langle j|\psi_t\rangle = \begin{cases} \frac{1}{ab}(e^{-it} + e^{\frac{it}{a-1}}(a-1) + a(b-1)) & \text{if } j = 0 \\ \frac{1}{ab}(e^{-it} + e^{\frac{it}{a-1}}(a-1) - a) & \text{if } 1 \leq j < b \\ \frac{1}{ab}(e^{-it} - e^{\frac{it}{a-1}}) & \text{otherwise} \end{cases} \tag{21}$$

For the distribution to be exactly uniform at time t, $P_j(t) = 1/(ab)$, for all j. This yields the condition $\sin^2(ta/[2(a-1)]) = \frac{ab}{4}$ or $1 \leq ab \leq 4$. There are only three *legal* (integral) cases, namely, $a = 1, b = 4$ (or $\overline{K_4}$), $a = b = 2$ (or $K_{2,2}$), and $a = 4, b = 1$ (or K_4). The case for the empty graph $\overline{K_4}$ is obvious, and we know from Theorem 1 that K_4 has uniform mixing. For the case of $K_{2,2}$, the three amplitude expressions are $\frac{1}{4}(e^{it} + e^{-it} + 2) = \frac{1}{2}(\cos(t) + 1)$, $\frac{1}{4}(e^{it} + e^{-it} - 2) = \frac{1}{2}(\cos(t) - 1)$, and $\frac{i}{2}\sin(t)$. For t being odd multiples of $\pi/2$, their probability forms achieve uniformity. So $K_{2,2}$ has uniform mixing.

Theorem 2 *No balanced complete multipartite graph, except for $K_{2,2}$, has the instantaneous exactly uniform mixing property under the continuous-time quantum walk model.*

For $K_{2,2}$, the average probabilities are $P(0) = P(1) = 3/8$ and $P(j) = 1/8$, for $j \neq 0, 1$. Hence, $K_{2,2}$ is also not average uniform mixing.

7. The complete cycle C_n

Let $H = \frac{1}{2}A$ be the normalized adjacency matrix of the complete cycle C_n on n vertices. Recall that $\omega^j = e^{2\pi ij/n}$, for $j = 0, 1, \ldots, n-1$. The eigenvalues of H are $\lambda_j = \frac{1}{2}(\omega^j + \omega^{j(n-1)}) = \cos(2\pi j/n)$. The wave equation of the continuous-time quantum walk is

$$|\psi_t\rangle = U_t|\psi_0\rangle = \frac{1}{n}\sum_{j=0}^{n-1} e^{-i\lambda_j t}|\omega_j\rangle = \frac{1}{n}\sum_{j=0}^{n-1} e^{-it\cos(2\pi j/n)}|\omega_j\rangle. \tag{22}$$

Thus, the wave amplitude at vertex k at time t is

$$\langle k|\psi_t\rangle = \frac{1}{n}\sum_{j=0}^{n-1} e^{-it\cos(2\pi j/n)}\omega^{jk}. \tag{23}$$

This is a complicated nested exponential sum.* Despite the fact that C_3 (which is equivalent to K_3) and C_4 (which is equivalent to $K_{2,2}$) both have the uniform mixing property, the general case of C_n, $n > 4$, remains intractable.†

Conjecture 1 *No complete cycle C_n, except for C_3 and C_4, has the instantaneous exactly uniform mixing property under the continuous-time quantum walk model.*

8. The Cayley graph of S_n

Let S_n be the symmetric group on n elements (the group of all permutations on $[n]$) and let T_n be the set of transpositions on $[n]$. The Cayley graph $X_n(S_n, T_n)$ is defined on the

*An alternative expression is $\langle k|\psi_t\rangle = \sum_{\nu \equiv \pm k \pmod{N}} (-i)^\nu J_\nu(t)$, where $J_\nu(t)$ is the Bessel function. This can be derived using techniques from Section III.C in [1].

†The discrete quantum walk on C_n has uniform mixing property [8].

vertex set S_n and $(\pi, \tau\pi)$ is an edge, for all $\pi \in S_n$ and $\tau \in T_n$; it is a bipartite, connected $\binom{n}{2}$-regular graph on $n!$ vertices. Consider the simplest case of S_3 with elements $\{e, (1\ 2), (1\ 3), (2\ 3), (1\ 2\ 3), (1\ 3\ 2)\}$. This Cayley graph on S_3 is isomorphic to $K_{3,3}$. By Theorem 2, the continuous-time quantum walk on it is not uniform mixing. We have verified that the same is true of S_4 via very pedestrian arguments. We conjecture that this phenomenon holds for all $n > 4$.

Conjecture 2 *No Cayley graph X_n, except for X_2, has the instantaneous exactly uniform mixing property under the continuous-time quantum walk model.*[‡]

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[‡]This conjecture was recently proved true by Gerhardt and Watrous [12].