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NON-UNIFORM MIXING OF QUANTUM WALK ON CYCLES

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A classical lazy random walk on cycles is known to mix with the uniform distribution. In contrast, we show that a continuous-time quantum walk on cycles exhibits strong non-uniform mixing properties. First, we prove that the *instantaneous* distribution of a quantum walk on most even-length cycles is never uniform. More specifically, we prove that a quantum walk on a cycle C_n is not instantaneous uniform mixing, whenever n satisfies either: (a) $n = 2^u$, for $u \geq 3$; or (b) $n = 2^u q$, for $u \geq 1$ and $q \equiv 3 \pmod 4$. Second, we prove that the *average* distribution of a quantum walk on any Abelian circulant graph is never uniform. As a corollary, the average distribution of a quantum walk on any standard circulant graph, such as the cycles, complete graphs, and even hypercubes, is never uniform. Nevertheless, we show that the average distribution of a quantum walk on the cycle C_n is $O(1/n)$-uniform.

Keywords: Quantum walk; continuous-time; mixing; circulant.

1. Introduction

Quantum walk on graphs is a non-trivial and interesting generalization of the classical random walk on graphs. A mathematical theory of both has proved to be relevant to physics, computer science, and more recently, to quantum information. An excellent survey of quantum walk on graphs is given by Kendon.[1] In this work, we will focus on continuous-time unitary quantum walk on finite graphs. Our goal is to show strong non-uniform mixing properties of a continuous-time quantum walk on cycles and circulant graphs, which demonstrates a distinct behavior from a classical lazy random walk on the same graphs.

A continuous-time quantum walk on a graph $G = (V, E)$ is defined using Schrödinger's equation by treating the adjacency matrix of G as the Hamiltonian of the quantum system. This treatment is standard in the physics literature (for example, see Ref. 2), where G is commonly known as an infinite low-dimensional lattice. This corresponds to a quantum analogue of the important investigations of classical random walks on $\mathbb{Z}^d$, for $d \geq 1$, by Polya and others (see Ref. 3).

Yet, the case when G is a finite graph has only been analyzed recently due to its potential applications in developing efficient quantum algorithms (see Refs. 4 and 5). An interesting mixing property of a continuous-time quantum walk on the hypercube graphs was observed by Moore and Russell.[6] They showed that a continuous-time quantum walk on the hypercube is instantaneous uniform mixing; that is, there are times when the probability distribution of the quantum walk, when measured, exactly equals the uniform distribution on the vertices of the hypercube. Although a classical random walk on the hypercube also mixes to uniform, a quantum walk hits the uniform distribution asymptotically faster.

Subsequent works showed that several other natural family of graphs do not share this uniform mixing property with the hypercube. For example, the complete graphs[7] and the Cayley graphs of the symmetric group[8] are known to be *not* instantaneous uniform mixing. However, there is a very natural class of graphs whose status remains open: the cycle graphs. Quantum walk on cycles has been studied in the discrete-time setting.[9,10] It is also known that the evolution of continuous-time quantum walk on cycles can be expressed as a summation involving Bessel functions (see Refs. 2 and 11). Still, it is unknown if a continuous-time quantum walk on cycles has the uniform mixing property.

In this work, we show that a continuous-time quantum walk on cycles exhibits strong non-uniform mixing properties. First, we prove that on most even-length cycles, the quantum walk is not instantaneous uniform mixing. The theorem applies to cycles whose lengths n are either a power of two, say, 2^u, where $u \geq 3$, or a product of a power of two and an odd number congruent to 3 modulo 4, that is, $n = 2^u q$, where $u \geq 1$ and $q \equiv 3 \pmod 4$. Our proof exploits spectral symmetries of even-length cycles coupled with some number-theoretic arguments. In a sense, our arguments only yield non-uniform mixing for *half* of the even lengths; a separate argument seems to be required for the case when $q \equiv 1 \pmod 4$.

Second, we consider average mixing of quantum walk on cycles. The notion of average mixing is a natural quantum generalization of stationary or limiting distributions in classical random walks on graphs. We prove a very general theorem stating that a continuous-time quantum walk on any Abelian group-theoretic circulant (defined in Ref. 12) is not average uniform mixing. Since the class of Abelian circulants include a natural family of graphs such as the cycles, complete graphs, and even hypercubes, as a corollary, we obtain the same non-uniform average mixing property for a continuous-time quantum walk on cycles. However, we also show that, in a quantum walk on cycles, the average distribution is $(1/n)$-close to uniform (in total variation distance). This property is not true for the family of complete graphs.

Our work heavily exploits the circulant structure and spectral properties of the underlying graphs. A more complete treatment of circulants and their beautiful theory is given by Davis[13] and Diaconis,[14] while a different aspect of quantum walk on circulant graphs is described by Saxena *et al.*[15]

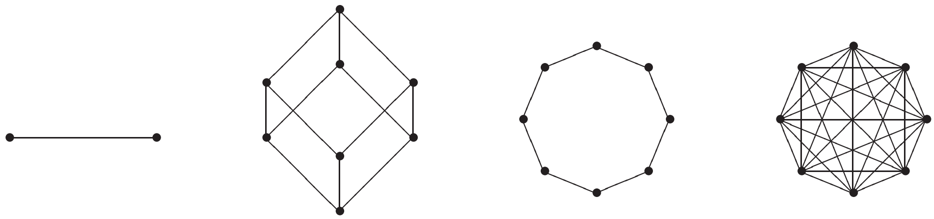
2. Preliminaries

For a logical statement S, let $[\![S]\!]$ denote the characteristic function of S which evaluates to 1 if S is true, and to 0 if it is false.

We only consider graphs $G = (V, E)$ that are simple, undirected, and connected. Let A_G be the adjacency matrix of G, where $A_G[j,k] = [\![(j,k) \in E]\!]$. A graph G is *circulant* if its adjacency matrix A_G is circulant. A circulant matrix A is specified by its first row, say $[a_0, a_1, \ldots, a_{n-1}]$, and is defined as $A[j,k] = a_{k-j \pmod n}$, where $j, k \in \mathbb{Z}_n$:

$$A = \begin{bmatrix} a_0 & a_1 & \cdots & a_{n-1} \\ a_{n-1} & a_0 & \cdots & a_{n-2} \\ \vdots & \vdots & \cdots & \vdots \\ a_1 & a_2 & \cdots & a_0 \end{bmatrix}. \tag{1}$$

Here $\mathbb{Z}_n$ denotes the group of integers $\{0, \ldots, n-1\}$ under addition modulo n. Note that $a_0 = 0$, since our graphs are simple, and $a_j = a_{n-j}$, since our graphs are



(a) (b) (c) (d)

Fig. 1. Some Abelian circulants and their quantum mixing properties. From left to right: (a) smallest circulant K_2; instantaneous and average uniform. (b) 3-cube or $\mathbb{Z}_2^3$-circulant; instantaneous but not average uniform (Moore and Russell[6]). (c) cycle C_8 or sparse $\mathbb{Z}_8$-circulant; not instantaneous uniform, but average $(1/n)$-uniform (this work). (d) the complete graph K_8 or dense $\mathbb{Z}_8$-circulant; neither instantaneous nor average $(1/n)$-uniform (Ahmadi *et al.*[7]).

undirected. Most known families of circulant graphs include the complete graphs and cycles (see Fig. 1).

All circulant graphs G are diagonalizable by the Fourier matrix F whose columns $|F_k\rangle$ are defined as $\langle j|F_k\rangle = \omega_n^{jk}/\sqrt{n}$, where $\omega_n = \exp(2\pi i/n)$:

$$F = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \omega_n & \omega_n^2 & \dots & \omega_n^{n-1} \\ 1 & \omega_n^2 & \omega_n^4 & \dots & \omega_n^{2(n-1)} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & \omega_n^{n-1} & \omega_n^{2(n-1)} & \dots & \omega_n^{(n-1)^2} \end{bmatrix}. \tag{2}$$

In fact, we have $FAF^{-1} = \sqrt{n} \cdot \mathrm{diag}(FA_0)$, for any circulant A, where $A_0 = A|0\rangle$ is the first column of A (see Refs. 13 and 16). This shows that the eigenvalues of A are given by

$$\lambda_j = \sum_{k=0}^{n-1} a_k\ \omega_n^{-jk}. \tag{3}$$

A *continuous-time quantum walk* on a graph $G = (V, E)$ is defined using the Schrödinger equation with the real symmetric matrix A_G as the Hamiltonian (see Farhi and Gutmann[4]). A classical random walk on a d-regular graph G is sensitive to the choice of the stochastic transition matrix: either $1/dA_G$, for the simple walk, or $1/2\, I + 1/2\, dA_G$, for the lazy walk. In our quantum walk, this choice is irrelevant since I and A_G commute, which implies that $e^{-it(\frac{1}{2}I+\frac{1}{2d}A_G)} = e^{-it/2}e^{-i(t/2d)A_G}$. The first term $e^{-it/2}$ is an irrelevant phase factor, while the second term involves a time shift $t/2d$ that may also be ignored. Thus, we may assume that our stochastic transition matrix is simply A_G. If $|\psi(t)\rangle \in \mathbb{C}^{|V|}$ is a time-dependent amplitude vector on the vertices of G, then the evolution of the quantum walk is given by

$$|\psi(t)\rangle = e^{-itA_G}|\psi(0)\rangle, \tag{4}$$

where $i = \sqrt{-1}$ and $|\psi(0)\rangle$ is the initial amplitude vector. The amplitude of the quantum walk of vertex j at time t is given by $\langle j|\psi(t)\rangle$. The *instantaneous* probability of vertex j at time t is $p_j(t) = |\langle j|\psi(t)\rangle|^2$. Let $P_t = \langle p_j(t) : j \in V\rangle$ be the instantaneous probability distribution of the quantum walk.

The *average* probability of vertex j is defined as

$$\overline{p}_j = \lim_{T\to\infty} \frac{1}{T}\int_0^T p_j(t)\ \mathrm{d}t. \tag{5}$$

The average probability distribution of the quantum walk will be denoted $\overline{P}$. This notion of average distribution (defined in Ref. 9 for discrete-time quantum walks) is similar to the notion of a stationary distribution in classical random walks.

Given two probability distributions P, Q on a finite set S, the *total variation distance* between P and Q is defined as $||P - Q|| = \sum_{s\in S} |P(s) - Q(s)|$. Let U be the uniform distribution on the vertices V of G. For a given $\varepsilon \geq 0$, we say that G is *instantaneous* ε-uniform *mixing* if there is a time t so that the total variation distance between P_t and U is at most ε, that is, $||P_t - U|| \leq \varepsilon$. We also say that G is *average ε-uniform mixing* if the total variation distance between $\overline{P}$ and U is at most ε, that is, $||\overline{P} - U|| \leq \varepsilon$. Whenever $\varepsilon = 0$, we say that *exact* uniform mixing is achieved.

For discrete-time quantum walk, Aharonov *et al.*[9] showed that a graph with distinct eigenvalues is potentially average uniform mixing. A continuous-time adaptation of this result is as follows. Suppose that G has eigenvalues $\lambda_0 \geq \cdots \geq \lambda_{n-1}$ with corresponding orthonormal eigenvectors $|z_0\rangle, \ldots, |z_{n-1}\rangle$. The average probability of vertex ℓ is

$$\overline{P}(\ell) = \lim_{T\to\infty} \frac{1}{T}\int_0^T |\langle \ell|e^{-itH}|\psi(0)\rangle|^2 \mathrm{d}t \tag{6}$$

$$= \sum_{j,k=0}^{n-1} \langle z_j|0\rangle\langle 0|z_k\rangle\langle \ell|z_j\rangle\langle z_k|\ell\rangle \lim_{T\to\infty}\frac{1}{T}\int_0^T e^{-it(\lambda_j-\lambda_k)}\mathrm{d}t. \tag{7}$$

Since $\lim_{T\to\infty} 1/T \int_0^T e^{-it\Delta}\mathrm{d}t = [\![\Delta = 0]\!]$, this implies that

$$\overline{P}(\ell) = \sum_{j,k=0}^{n-1} \langle z_j|0\rangle\langle 0|z_k\rangle\langle \ell|z_j\rangle\langle z_k|\ell\rangle [\![\lambda_j = \lambda_k]\!]. \tag{8}$$

Moreover, if all eigenvalues are distinct, then $\overline{P}(\ell) = \sum_{j=0}^{n-1} |\langle \ell|z_j\rangle|^2 |\langle z_j|0\rangle|^2$.

3. Non-Uniform Instantaneous Mixing of Even-Length Cycles

In this section, we show that a continuous-time quantum walk on most even-length cycles C_n is not instantaneous uniform mixing. Using Eq. (3), the eigenvalues of a cycle C_n are given by

$$\lambda_k = 2\cos(2\pi k/n), \quad k = 0, \ldots, n-1. \tag{9}$$

Note that $\lambda_0 = 2$, $\lambda_{n-k} = \lambda_k$, for $1 \leq k < n/2$, and $\lambda_{n/2} = -2$, when n is even. Let $|\psi_n(t)\rangle$ describe a continuous-time quantum walk on C_n starting at vertex 0. If A is the circulant adjacency matrix of C_n, then

$$|\psi_n(t)\rangle = e^{-iAt}|0\rangle = e^{-iAt} \sum_{k=0}^{n-1} \frac{1}{\sqrt{n}}|F_k\rangle = \frac{1}{\sqrt{n}} \sum_{k=0}^{n-1} e^{-i\lambda_k t}|F_k\rangle. \tag{10}$$

This shows that, for each $j = 0, \ldots, n-1$, we have

$$\langle j\psi_n(t)\rangle = \frac{1}{n} \sum_{0 \leq k < n} e^{-i\lambda_k t}\omega_n^{jk}. \tag{11}$$

Fact 1. Let $|\psi_n(t)\rangle$ describe a continuous-time quantum walk on C_n, where n is even. Then, for any $j = 0, \ldots, n-1$, we have

$$\langle j|\psi_n(t)\rangle = \frac{1}{n} \left\{ e^{-2it} + (-1)^j e^{2it} + 2 \sum_{1 \leq k < n/2} e^{-i\lambda_k t} \cos(2\pi jk/n) \right\}. \tag{12}$$

Proof. Using the eigenvalue symmetry $\lambda_k = \lambda_{n-k}$, for $1 \leq k < n/2$, combined with Eq. (11), yields the claim. □

The following lemma shows that some properties of a quantum walk on C_n can be deduced from a quantum walk on C_m, if m divides n. This reduction will be helpful in analyzing a quantum walk on even-length cycles.

Lemma 2. *Let $m, n > 0$ be integers so that $m|n$. Then, for each $0 \leq a < m$ we have*

$$\sum_{0 \leq j < n} [\![j \equiv a \pmod{m}]\!] \langle j|\psi_n(t)\rangle = \langle a|\psi_m(t)\rangle. \tag{13}$$

Proof. Using Eq. (11), after switching summations, we get:

$$\sum_{0 \leq j < n} [\![j \equiv a \pmod{m}]\!] \langle j|\psi_n(t)\rangle = \frac{1}{n} \sum_{0 \leq k < n} e^{-i\lambda_k t} \sum_{0 \leq j < n} [\![j \equiv a \pmod{m}]\!] \times \omega_n^{jk}. \tag{14}$$

Rewriting the inner index j as $m\tilde{j} + a$, as $\tilde{j}$ varies in $0 \leq \tilde{j} < n/m$, we get (after renaming $\tilde{j}$ back to j):

$$\frac{1}{n} \sum_{0 \leq k < n} e^{-i\lambda_k t} \sum_{0 \leq j < n/m} \omega_n^{(mj+a)k} = \frac{1}{n} \sum_{0 \leq k < n} e^{-i\lambda_k t}\omega_n^{ak} \sum_{0 \leq j < n/m} \omega_{n/m}^{jk}. \tag{15}$$

Next, we note that $\sum_{j=0}^{n-1} \omega_n^j = n \times [\![k \equiv 0 \pmod{n}]\!]$. This yields:

$$\frac{1}{m} \sum_{0 \leq k < n} [\![k \equiv 0 \pmod{n/m}]\!] \times e^{-i\lambda_k t}\omega_n^{ak} = \frac{1}{m} \sum_{0 \leq k < m} e^{-i\lambda_k t}\omega_m^{ak}, \tag{16}$$

which equals $\langle a|\psi_m(t)\rangle$. □

A quantum walk on C_2, which is a multigraph on two vertices with two distinct edges connecting the vertices, is given by:

$$|\psi_t\rangle = \exp\left(-it\begin{bmatrix}0 & 2\\ 2 & 0\end{bmatrix}\right)|0\rangle = \frac{1}{2}\left\{e^{-2it}\begin{bmatrix}1\\1\end{bmatrix} + e^{2it}\begin{bmatrix}1\\-1\end{bmatrix}\right\} = \begin{bmatrix}\cos(2t)\\ -i\sin(2t)\end{bmatrix}. \quad (17)$$

Thus, we have $P_t = \begin{bmatrix}\cos^2(2t) & \sin^2(2t)\end{bmatrix}^T$. Applying the previous lemma to even-length cycles, a quantum walk on C_{2n} behaves in a similar manner to a quantum walk on a 2-vertex cycle. More specifically, the sum of the amplitudes on the vertices with even (respectively, odd) indices in a quantum walk on C_{2n} corresponds exactly to the amplitude of vertex 0 (respectively, 1) in a quantum walk on C_2.

Corollary 3. *Let $|\psi_n(t)\rangle$ describe a continuous-time quantum walk on C_n, where n is even. Then,*

$$\sum_{0\leq j<n/2}\langle 2j|\psi_n(t)\rangle = \cos(2t), \qquad \sum_{0\leq j<n/2}\langle 2j+1|\psi_n(t)\rangle = -i\sin(2t). \quad (18)$$

Proof. Since n is even, apply Lemma 2 with $m = 2$. □

A further eigenvalue symmetry on even-length cycles yields a useful simplification on the amplitude expression given by Fact 1.

Lemma 4. *Let $|\psi_n(t)\rangle$ describe a continuous-time quantum walk on C_n, where n is even. Then,*

$$\langle j|\psi_n(t)\rangle = \frac{1}{n}\left\{\varepsilon_{j,0}^{(n)}(t) + 2\sum_{1\leq k<n/4}\varepsilon_{j,k}^{(n)}(t)\cos(2\pi jk/n) + 2\delta_j^{(n)}\right\}, \quad (19)$$

where $\varepsilon_{j,k}^{(n)}(t) = e^{-i\lambda_k t} + (-1)^j e^{i\lambda_k t}$, and $\delta_j^{(n)} = [\![4|n \text{ and } 2|j]\!](-1)^{j/2}$.

Proof. Using Fact 1 and the eigenvalue symmetry $\lambda_{n/2-k} = -\lambda_k$, for $1\leq k<n/4$, we obtain the following expression for $\langle j|\psi_n\rangle(t)$:

$$\frac{1}{n}\left\{e^{-2it} + (-1)^j e^{2it} + 2\sum_{1\leq k<n/4}(e^{-i\lambda_k t} + (-1)^j e^{i\lambda_k t})\cos\left(\frac{2\pi jk}{n}\right) + 2\delta_j^{(n)}\right\} \quad (20)$$

since $\cos(2\pi j(n/2-k)/n) = (-1)^j\cos(2\pi jk/n)$. The term involving $\delta_j^{(n)}$ exists only when n is divisible by 4 and has the value of $e^{-i\lambda_{n/4}}\cos(j\pi/2) = [\![2|j]\!](-1)^{j/2}$, since $\lambda_{n/4} = 0$. □

Using the previous lemma, we may deduce that the amplitude values on the vertices in a quantum walk on an even-length cycle are purely real or purely imaginary; moreover, this is completely determined by the parity of the vertex index.

Corollary 5. *Let $|\psi_n(t)\rangle$ describe a continuous-time quantum walk on C_n, where n is even. Then, $\langle j|\psi_n(t)\rangle$ is a real number, if j is even, and is an imaginary number, if j is odd.*

Proof. Using Lemma 4, we note that $e^{-i\lambda_k t} + (-1)^j e^{i\lambda_k t}$ equals $2\cos(\lambda_k t)$, whenever j is even, and equals $-2i\sin(\lambda_k t)$, if j is odd. Also, note that the term $\delta_j^{(n)}$ is always real and is non-zero only when j is even. □

Next, we show a lemma which connects the sum of amplitudes on a pair of vertices in a quantum walk on C_{2n} to the amplitude on a single vertex in a quantum walk on C_n. This lemma will be useful in deducing the type of amplitude expressions involved in a quantum walk on C_{2^u}, for some $u \geq 1$.

Lemma 6. *Let $|\psi_n(t)\rangle$ describe a continuous-time quantum walk on C_n, where n is even. Then, for all $0 \leq j < n$, we have*

$$\langle j|\psi_{2n}(t)\rangle + \langle n-j|\psi_{2n}(t)\rangle = \langle j|\psi_n(t)\rangle. \tag{21}$$

Proof. Note that $\cos(2\pi(n-j)k/(2n)) = (-1)^k \cos(2\pi jk/(2n))$. By Lemma 4, the sum $\langle j|\psi_{2n}(t)\rangle + \langle n-j|\psi_{2n}(t)\rangle$ equals

$$\frac{1}{n}\left\{\varepsilon_{j,0}^{(2n)}(t) + 2\sum_{1\leq k<n/2} [\![k \text{ even}]\!] \cos\left(\frac{2\pi jk}{2n}\right)\varepsilon_{j,k}^{(2n)}(t)\right\}. \tag{22}$$

Since $\varepsilon_{j,2k}^{(2n)}(t) = \varepsilon_{j,k}^{(n)}(t)$, we get

$$\frac{1}{n}\left\{\delta_{j,0}^{(n)} + 2\sum_{1\leq k<n/4} \cos(2\pi jk/n)\varepsilon_{j,k}^{(n)}(t)\right\}. \tag{23}$$

Again by Lemma 4, the last expression equals $\langle j|\psi_n(t)\rangle$. □

Finally, we are ready to state and prove a theorem showing that a continuous-time quantum walk with most even-length cycles is *not* instantaneous exactly uniform mixing. The proof uses several observations stated in the previous lemmas.

Theorem 7. *The family of cycles C_n is not instantaneous uniform mixing, where n satisfies either* (a) $n = 2^u$, *where* $u \geq 3$; *or* (b) $n = 2^u q$, *where* $u \geq 1$ *and* $q \equiv 3 \pmod 4$.

Proof. Assume that there is a time t for which $|\langle j|\psi(t)\rangle|^2 = 1/n$. By Corollary 5, we have

$$\langle j|\psi(t)\rangle = \begin{cases} \pm 1/\sqrt{n} & \text{if } j \text{ is even} \\ \pm i/\sqrt{n} & \text{if } j \text{ is odd.} \end{cases} \tag{24}$$

Also, we have

$$\cos(2t) = \sum_{0\le j<n/2} \langle 2j|\psi(t)\rangle = \frac{n}{2}\frac{1}{\sqrt{n}} - \frac{2k}{\sqrt{n}} = \frac{(n-4k)}{2\sqrt{n}}, \tag{25}$$

where k is the number of j's for which $\langle 2j|\psi(t)\rangle$ is negative. Similarly, we have

$$-i\sin(2t) = \frac{(n-4\ell)}{2\sqrt{n}}, \tag{26}$$

where ℓ is the number of j's for which $\langle 2j+1|\psi(t)\rangle$ is negative. Since $\cos^2(2t) + \sin^2(2t) = 1$, we obtain

$$(n-4k)^2 + (n-4\ell)^2 = 4n. \tag{27}$$

Let $a_k = n-4k$ and $a_\ell = n-4\ell$. There are two cases to consider: one of a_k or a_ℓ is zero, or both are non-zero.

If one of them is zero, say $a_k = 0$, then $a_\ell^2 = 4n$. If $n = 2^u q$, where $u \ge 1$ and $q \equiv 3\,(\mathrm{mod}\ 4)$, we have a contradiction since $2^u q$ is not a square, if u is odd or $q \equiv 3\,(\mathrm{mod}\ 4)$. Otherwise, u is even and $q = 1$, and, by repeated applications of Lemma 6, we observe that $\langle 0|\psi_8(t)\rangle = a/\sqrt{n} = a/2^m$, for some integers $a, m \in \mathbb{Z}$. But, by Lemma 4, we have

$$\langle 0|\psi_8(t)\rangle = \frac{1}{4}\cos(2t) + \frac{1}{2}\cos(\sqrt{2}t). \tag{28}$$

Since $\cos(t) = 0$ or $\sin(t) = 0$ in this case, we must have $t = k(\pi/2)$, for some $k \in \mathbb{Z}$. However, $\cos(k\pi/\sqrt{2})$ is not rational, for any integer k, since $(e^{i(\pi/2)\sqrt{2}})^k$ is transcendental, by the Gelfond-Schneider[a] theorem (see Ref. 17).

Next, we consider the case when both a_k and a_ℓ are non-zero. If both terms are odd, then considering Eq. (27), the left-hand size satisfies $a_k^2 + a_\ell^2 \equiv 2(\mathrm{mod}\ 4)$ whereas the right-hand side satisfies $4n \equiv 0\,(\mathrm{mod}\ 4)$; this is a contradiction. Otherwise, if both terms are even, then a factor of 4 can be removed from both sides of Eq. (27). Continuing this process, we arrived at a case where either the right-hand side is $q \equiv 3\,(\mathrm{mod}\ 4)$ or both a_k and a_ℓ are odd. In either case, we arrive at a contradiction modulo 4.

This completes the proof of the theorem. $\square$

4. Non-Uniform Average Mixing on Abelian Circulants

Our main theorem in this section shows that the average distribution of a continuous-time quantum walk on any cycle, except for C_2, is never uniform. In fact, we prove a much stronger theorem stating that the average distribution of a continuous-time quantum walk on any $\mathcal{G}$-circulant, for any Abelian group $\mathcal{G}$ (as defined in Ref. 12) is never uniform, except for C_2.

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[a]The Gelfond-Schneider theorem states that α^β is transcendental, if α and β are algebraic numbers with $\alpha \neq 0$ and $\alpha \neq 1$, and if β is not a real rational number.

Diaconis[12] described the following interesting group-theoretic generalization of circulants. Let $\mathcal{G}$ be a group of order n and let $f : \mathcal{G} \to \mathbb{C}$ be a *class* function of $\mathcal{G}$ (that is, it is constant on the conjugacy classes of $\mathcal{G}$). Consider the matrix $M_{\mathcal{G}}^{f}$ defined on $\mathcal{G} \times \mathcal{G}$ as $M_{\mathcal{G}}^{f}[s,t] = f(st^{-1})$. Note that with $\mathcal{G}$ being the cyclic group $\mathbb{Z}_n$ of order n, we recover the standard circulant graphs, whereas with $\mathcal{G} = \mathbb{Z}_2^n$, we obtain the hypercube graphs.

Let $\rho : \mathcal{G} \to GL(n, \mathbb{C})$ be a representation of $\mathcal{G}$ with dimension n. The Fourier transform of f at a representation ρ is defined as

$$\hat{f}(\rho) = \sum_{x \in \mathcal{G}} f(x)\rho(x). \tag{29}$$

As usual, Fourier inversion reconstructs f from its Fourier transform at all irreducible representations $\rho_1, \ldots, \rho_m$ of $\mathcal{G}$ with dimensions $d_1, \ldots, d_m$, respectively:

$$f(x) = \frac{1}{|\mathcal{G}|} \sum_{j=1}^{m} d_j \mathrm{Trace}(\rho_j(x^{-1})\hat{f}(\rho_j)). \tag{30}$$

For each irreducible representation ρ_j, we define a $d_j^2 \times d_j^2$ block matrix D_j as $D_j = \mathrm{diag}(\hat{f}(\rho_j))$. Next, let $D = \mathrm{diag}(D_1, \ldots, D_h)$ be a $|\mathcal{G}| \times |\mathcal{G}|$ matrix, since $|\mathcal{G}| = \sum_{j=1}^{m} d_j^2$. Also, we define the vector ψ_j of length d_j^2 as $\psi_j(x) = (\sqrt{d_j})/(|\mathcal{G}|)\langle \rho_j(x)[s,t] : 1 \leq s,t \leq d_j \rangle$ and the vector $\psi(x) = \langle \psi_j(x) : 1 \leq j \leq m \rangle$ of length $|\mathcal{G}|$. Finally, we define the matrix $\mathcal{X} = [\psi(x_1) \ldots \psi(x_n)]$, where $x_1, \ldots, x_n$ are the elements of $\mathcal{G}$.

Theorem 8 (Diaconis[12]). *If $f : \mathcal{G} \to \mathbb{C}$ is a class function of a finite group $\mathcal{G}$, then $M_{\mathcal{G}}^{f}$ is* unitarily diagonalized *by $\mathcal{X}$, that is, $M_{\mathcal{G}}^{f} = \mathcal{X}^{\dagger} D \mathcal{X}$, where, for each $j = 1, \ldots, m$, we have $D_j = \lambda_j I_{d_j^2}$, $\chi_j(x) = \mathrm{Trace}(\rho_j(x))$ is the character of ρ_j at x, and the eigenvalue is*

$$\lambda_j = \frac{1}{d_j} \sum_{x \in \mathcal{G}} f(x)\overline{\chi_j}(x). \tag{31}$$

We are interested in applying Theorem 8 for an Abelian group $\mathcal{G}$, where all of its group representations have dimension one. Our main result shows that the spectral gap of $M_{\mathcal{G}}^{f}$, for any Abelian group $\mathcal{G}$, is zero. This shows that average uniform mixing is impossible.

The Hadamard matrix H_n (of Sylvester type) is defined recursively as:

$$H_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad \text{and} \quad H_n = \begin{bmatrix} H_{n-1} & H_{n-1} \\ H_{n-1} & -H_{n-1} \end{bmatrix}, \quad n > 2. \tag{32}$$

We call graph G a *Hadamard* circulant if it is diagonalized by some Hadamard matrix H_n. Alternatively, these are $\mathcal{G}$-circulant matrices for $\mathcal{G} = \mathbb{Z}_2^n$. Although Eq. (8) suggests that a graph with distinct eigenvalues diagonalized by Hadamard matrices might be average uniform mixing, the following lemma disproves this possibility.

Lemma 9. *Let G be a graph diagonalized by a Hadamard matrix H_n, for $n > 2$. Then G has spectral gap zero.*

Proof. Consider the characters of $\mathbb{Z}_2^n$ defined for each $a \in \mathbb{Z}_2^n$ as $\chi_a(x) = \prod_{j=1}^n (1 - 2a_j x_j)$. From Eq. (31), we get $\lambda_a = \sum_{x \in \mathbb{Z}_2^n} f(x)\chi_a(x)$, where $f : \mathbb{Z}_2^n \to \{0, 1\}$ defines the first column of the adjacency matrix of G. Let $|f| = \{x \neq 0_n : f(x) = 1\}$. Assume that $|f| < 2^n - 1$, otherwise we get the complete graph which has only 2 distinct eigenvalues. If $|f|$ is even, then $\lambda_a \in \{0, \pm 2, \ldots, \pm|f|\}$. Since the eigenvalues can take at most $|f| + 1 < 2^n$ values, by the pigeonhole principle, there exist two non-distinct eigenvalues. If $|f|$ is odd, then $\lambda_a \in \{\pm 1, \pm 3, \ldots, \pm|f|\}$. Similarly, the eigenvalues range on at most $|f| < 2^n - 1$ values, and again there exist two non-distinct eigenvalues. □

Theorem 10. *For any Abelian group $\mathcal{G}$, no $\mathcal{G}$-circulant, except for C_2, is average uniform mixing.*

Proof. Let $\mathcal{G} = \mathbb{Z}_{n_1} \times \cdots \times \mathbb{Z}_{n_k}$ be an Abelian group. If all elements of $\mathcal{G}$ have order 2 (except for the identity), we appeal to Lemma 9. Otherwise, fix $a \in \mathcal{G}$ with order greater than 2. The character corresponding to a is $\chi_a(x) = \prod_{j=1}^k \chi_{a_j}(x_j)$. From Eq. (31),

$$\lambda_a = \sum_{x \neq 0} f(x)\overline{\chi}_a(x) = \sum_{x \neq 0} f(x)\overline{\chi}_{-a}(-x) = \sum_{x \neq 0} f(-x)\overline{\chi}_{-a}(-x) = \lambda_{-a}. \tag{33}$$

Thus, the spectral gap of $M_{\mathcal{G}}^f$ is zero. Finally, since $\mathcal{G}$ is Abelian, its characters are complex roots of unity; thus, applying Eq. (8), we obtain the claim. □

The above theorem implies that the n-cube and the standard circulant graphs are not average uniform mixing, as stated in the following corollary.

Corollary 11. *No $\mathbb{Z}_2^n$-circulant and no $\mathbb{Z}_n$-circulant, except for C_2, is average uniform mixing.*

Next, we relax our requirement of exact uniform average mixing and allow mixing to be $(1/n)$-uniform. We observe that the cycle graphs and the complete graphs behave differently with respect to average near uniform mixing.

Theorem 12. *The cycle C_n is average $(1/n)$-uniform mixing.*

Proof. Let $\omega = \exp(2\pi i/n)$. Using Eq. (8) for circulants, we have

$$\overline{P}(\ell) = \frac{1}{n^2} \sum_{j,k=0}^{n-1} \omega^{(j-k)\ell} [\![\lambda_j = \lambda_k]\!] = \frac{1}{n} + \frac{1}{n^2} \sum_{j \neq k} \omega^{(j-k)\ell} [\![\lambda_j = \lambda_k]\!]. \tag{34}$$

A result of Diaconis and Shahshahani (see Ref. 14) states that $||\overline{P} - U|| \leq 1/4 \sum_\rho |\widehat{\overline{P}}(\rho)|^2$, where the sum is over non-trivial irreducible representations. The characters of $\mathbb{Z}_n$ are given by $\chi_a(x) = \omega^{ax}$, and thus, for $a \neq 0$,

$$\widehat{\overline{P}}(a) = \sum_\ell \overline{P}(\ell)\chi_a(\ell) = \frac{1}{n^2} \sum_{j \neq k:\ \lambda_j = \lambda_k} \sum_\ell \omega^{(j-k+a)\ell} = \frac{1}{n}. \tag{35}$$

The last equality holds because there is a unique pair (j, k) such that $j - k + a = 0$; this pair contributes n to the sum while the other pairs contribute 0 to the sum. Therefore, $||\overline{P} - U|| \leq (n-1)/4n^2 < 1/4n$. □

In contrast, the average distribution of a quantum walk on the complete graphs K_n is not near uniform.

Theorem 13 (Ahmadi *et al.*[7]). *The complete graph K_n is not average $(1/n)$-uniform mixing.*

Proof. As shown in Ref. 7, for $\ell \neq 0$, we have $\overline{P}(\ell) = 2/n^2$, and $\overline{P}(0) = 1 - 2(n-1)/n^2$. Thus $||\overline{P} - U|| = 2(1 - 1/n)(1 - 2/n) \gg 1/n$. □

5. Conclusions

In this work, we have shown that a continuous-time quantum walk on cycles exhibits strong non-classical mixing characteristics. First, we prove that a continuous-time quantum walk on most even-length cycles is not instantaneous uniform mixing. This partially settles a conjecture made in Ref. 7. Second, we prove that a continuous-time quantum walk on any cycle is not average uniform mixing. The latter result is obtained as a corollary of a stronger theorem for a continuous-time quantum walk on any Abelian circulant graph. This class of graphs include the natural families of cycles, complete graphs, hypercubes, and others. In contrast, classical lazy random walks on the same graphs mix to the uniform distribution.

We leave the case of the odd-length cycles as well as cycles of length $2^u q$, with $u \geq 1$ and $q \equiv 1 (\mathrm{mod}\ 4)$, for future work. Also, we are curious to investigate if there is something interesting about the quantum mixing status of prime-length cycles. Finally, the only known class of graphs with instantaneous uniform mixing is the hypercube family, and the only graph known to be average uniform mixing is the connected two-vertex graph. It is conceivable that these are *the* two lone examples of uniform mixing in circulants.

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