Quantum Information and Computation, Vol.6, No.4&5 (2006) 370–381

MIXING OF QUANTUM WALK ON CIRCULANT BUNKBEDS

PETER LO
Dept. Mathematics and Computer Science, St. Mary's College of Maryland
St. Mary's City, MD 20686 USA

SIDDHARTH RAJARAM*
Dept. Mathematics, Middlebury College, VT 05753 USA

DIANA SCHEPENS
Dept. Mathematics and Computer Science, Houghton College, Houghton, NY 14744 USA

DANIEL SULLIVAN
Dept. Mathematics and Statistics, Swarthmore College, Swarthmore, PA 19081 USA

CHRISTINO TAMON†
Dept. Computer Science and Center for Quantum Device Technology,
Clarkson University, Potsdam, NY 13699 USA

JEFFREY WARD
Div. Mathematics and Computer Science, Clarkson University, Potsdam, NY 13699 USA

Received September 9, 2005
Revised December 20, 2005

This paper gives new observations on the mixing dynamics of a continuous-time quantum walk on circulants and their bunkbeds. These bunkbeds are defined through two standard graph operators: the *join* $G + H$ and the *Cartesian product* $G \times H$ of graphs G and H. Our results include the following: (i) The quantum walk is average uniform mixing on circulants with bounded eigenvalue multiplicity; this extends a known fact about the cycles C_n. (ii) Explicit analysis of the probability distribution of the quantum walk on the join of circulants; this explains why complete multipartite graphs are not average uniform mixing, using the fact $K_n = K_1 + K_{n-1}$ and $K_{n,\ldots,n} = \overline{K}_n + \ldots + \overline{K}_n$. (iii) The quantum walk on the Cartesian product of a m-vertex path P_m and a circulant G, namely, $P_m \times G$, is average uniform mixing if G is; this highlights a difference between circulants and the hypercubes $Q_n = P_2 \times Q_{n-1}$. Our proofs employ purely elementary arguments based on the spectra of the graphs.

Keywords: Quantum walks, continuous-time, mixing, circulants
Communicated by: R Cleve & J Watrous

1. Introduction

The study of continuous-time quantum walks on graphs has important potential applications in quantum computation [16]. First, as an algorithmic technique, it was used to devise efficient quantum search algorithms with considerable speedup over classical algorithms [7]. Second,

*Contact author: srajaram@middlebury.edu, siddharth.rajaram@gmail.com
†Contact author: tino@clarkson.edu

it may provide a simpler physical implementation of a quantum computer, given that there is an abundance of physical processes that simulate quantum walk on graphs [9]. In the physics literature, continuous-time quantum walks are mainly studied over infinite constant-dimensional lattices, such as the one-dimensional line (see [10], Chapters 13,16). On the other hand, the study of random walks on general graphs is a topic of broad interest in the mathematics and computer science community [6, 14].

In this paper, we study the mixing dynamics of continuous-time quantum walks on circulant graphs. More particularly, we consider the *average* or limiting probability distribution of a quantum walk. This notion was introduced in [1] and is the quantum analogue of a stationary distribution of classical random walks. On the circulant graphs, our goal was to characterize the graphs for which the continuous-time quantum walk reaches (almost) uniform average probability distribution. It was previously known that cycles are near uniform mixing, whereas the complete graphs and hypercubes are not (see [2, 15]). Our other goal in this paper is to discover graph theoretic structures that may explain this polarized phenomena.

First, we show that circulants with bounded eigenvalue multiplicity are almost uniform mixing. This generalization explains why cycles are uniform mixing. Second, we consider bunkbed graphs constructed using the join and the Cartesian product operators. By analyzing the join of two circulants, we observe an interesting mixing phenomena on the cone $K_1 + G$ of a circulant G, that is dependent on the density of G. If the quantum walk starts on K_1, a dense graph G *repels* the probability away from the copy of G. This explains why the limiting distribution of a quantum walk on the complete graph is not near the uniform distribution. We extend this investigation to the homogeneous join of circulants, namely, $G + \ldots + G$, for a circulant G. We show that this bunkbed graph is uniform mixing if G is uniform mixing and the join is over a constant number of copies of G. A corollary of this transference property explains the non-uniform mixing of the complete multipartite graphs $\overline{K}_n + \ldots + \overline{K}_n$.

We also analyze bunkbed graphs obtained from the Cartesian product $P_m \times G$ of a path P_m and a circulant G. On this bunkbed structure, we observe another transference property: the quantum walk on $P_m \times G$ is uniform mixing if it is uniform mixing on G and the path is of constant size. This highlights a striking difference with the hypercube Q_n, since the hypercube is also a bunkbed $Q_n = P_2 \times Q_{n-1}$, but it is known that they are not uniform mixing [15]. It is interesting to note that both classes of graphs are group-theoretic circulants (see [8]), since our circulants are the $\mathbb{Z}_n$-circulants while hypercubes are the $(\mathbb{Z}_2)^n$-circulants. This suggests a group theoretic investigation into the mixing phenomena of generalized circulants, which we leave for future work.

In this paper, we focus exclusively on continuous-time quantum walks. We refer the reader to [12] for a survey of other models of quantum walks. As a final remark, we mention that most of the graphs we consider have the standard stationary distributions in the classical random walks where the limiting probability of a vertex is proportional to its degree [4].

2. Preliminaries

For a graph $G = (V, E)$, let A_G be the adjacency matrix of G, where $A_G[j,k] = [\![(j,k) \in E]\!]$. Here and throughout, we will use $[\![\Psi]\!]$ to denote the characteristic function of a logical statement Ψ, that is, 1 if Ψ is true, and 0 if it is false. We consider simple, undirected graphs that are connected, and mostly regular. A graph G is *simple* if A_G has zeros on its diagonal,

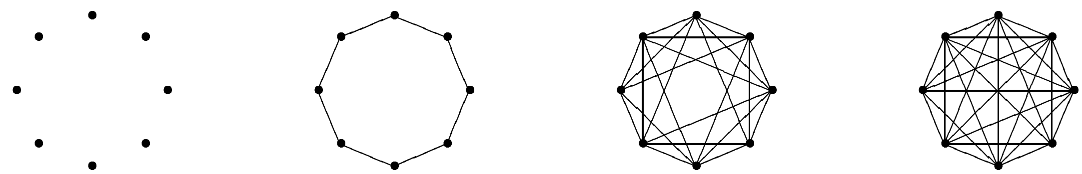

Fig. 1. Examples of circulants of order 8. From left to right: (i) the empty graph $\overline{K}_8$. (ii) the cycle C_8. (iii) the 6-regular circulant of order 8. (iv) the complete graph K_8.

is *undirected* if A_G is symmetric, is *connected* if A_G^k is the all-one matrix, for some finite k, and is d-regular if each row of A_G has exactly d ones. The set of eigenvalues of A_G is denoted $Sp(G)$, and the (algebraic) multiplicity of an eigenvalue λ is denoted $m(\lambda)$. The spectral *type* $\tau(G)$ of a graph G is the number of distinct eigenvalues of the adjacency matrix A_G of G. We will denote the maximum (algebraic) multiplicity of any eigenvalue of graph G by $\mu(G)$. Further background on graph theory can be found in [6, 5, 13].

We briefly describe several graph operators that we will use in this paper. The *complement* $\overline{G}$ of a graph $G = (V, E)$ is the graph with $V(\overline{G}) = V$ and $E(\overline{G}) = \{(x, y) : (x, y) \notin E\}$. The (disjoint) *union* $G \cup H$ is the graph defined over $V(G \cup H) = V(G) \cup V(H)$ with $E(G \cup H) = E(G) \cup E(H)$. The *join* $G + H$ is defined so as to satisfy $\overline{G + H} = \overline{G} \cup \overline{H}$ (see [17]). The Cartesian product $G \times H$ is defined over the vertex set $V(G) \times V(H)$, where $((g_1, h_1), (g_2, h_2))$ is an edge if either $g_1 = g_2$ and $(h_1, h_2) \in E(H)$, or $h_1 = h_2$ and $(g_1, g_2) \in E(G)$. Some of the families of graphs that we will consider include the cycles C_n, the paths P_n, the complete multipartite graphs $K_n^{(m)} = \sum_{j=1}^{m} \overline{K}_n$ (which includes the complete graphs K_n), and the hypercubes $Q_n = P_2 \times Q_{n-1}$, for $n > 2$, where $Q_1 = P_2$.

A graph G is called *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 $j, k \in \mathbb{Z}_n$. 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 undirected. Connectivity is guaranteed if the greatest common divisor of n and all indices k, for which $a_k = 1$, is one. Alternatively, a circulant graph $G = (V, E)$ can be specified by a subset $S \subseteq \mathbb{Z}_n$, where $(j, k) \in E$ if $k - j \in S$. In this case, we write $G = \langle S \rangle$. We will assume that S is closed under taking inverses, namely, if $d \in S$, then $-d \in S$. Figure 1 contains some examples of circulant graphs.

It is known that circulant graphs G are diagonalizable by the Fourier matrix F defined as $F_{j,k} = n^{-1/2}\omega_n^{jk}$, where $\omega_n = \exp(2\pi i/n)$. In fact, the eigenvalues of A_G are

$$\lambda_j = \sum_{k=1}^{n-1} a_k \omega^{jk} = \sum_{k=1}^{\lfloor (n-1)/2 \rfloor} 2\cos\left(\frac{2\pi jk}{n}\right) \; + \; [\![n \text{ even}]\!] \; a_{n/2} \; (-1)^j. \tag{1}$$

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 [7]). 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

$$|\psi(t)\rangle = e^{-itA_G}|\psi(0)\rangle, \tag{2}$$

where $i = \sqrt{-1}$ and $|\psi(0)\rangle$ is the initial amplitude vector. We usually assume that $|\psi(0)\rangle$ is a unit vector, with $\langle x|\psi(0)\rangle = [\![x = v_0]\!]$, for some start vertex v_0. The amplitude of the quantum walk on vertex j at time t is given by $\psi_j(t) = \langle j|\psi(t)\rangle$, while the probability of being on vertex j at time t is $p_j(t) = |\psi_j(t)|^2$. The average (or limiting) probability of being on vertex j is defined as

$$\overline{p}_j = \lim_{T\to\infty} \frac{1}{T}\int_0^T p_j(t)\ \mathsf{d}t. \tag{3}$$

This notion appeared in [1] in the context of discrete-time quantum walks. The limiting probability distribution of the quantum walk will be denoted $\overline{P}$.

Definition 1 *(Average Uniform Mixing)*
The average mixing of a continuous-time quantum walk on a graph $G = (V,E)$ is called uniform *if $\overline{p}_j = O(1/|V|)$, for each vertex j of G.*

Remark Note that in the above definition, we only require that each limiting probability be linearly proportional to the uniform probability value. This is less stringent than requiring that the quantum walk achieves *exactly* uniform probability distribution (see [3, 2]). When the graph G is not regular, the limiting probability distribution $\overline{P}$ may depend on the initial state $|\psi(0)\rangle$. We will specify carefully the effect of the initial states in these cases, but suppress this dependence for vertex-transitive graphs.*

3. Mixing and Bounded Multiplicities

Theorem 1 *Let G be a circulant graph. If $\mu(G)$ is bounded, then the continuous-time quantum walk on G is average uniform mixing.*

Proof Let n be the order of G and let A be the adjacency matrix of G. Since $|0\rangle = \sum_{k=0}^{n-1} \frac{1}{\sqrt{n}}|F_k\rangle$, if $|\psi(0)\rangle = |0\rangle$, we have $|\psi(t)\rangle = e^{-itA}|\psi(0)\rangle = \frac{1}{\sqrt{n}}\sum_{k=0}^{n-1} e^{-it\lambda_k}|F_k\rangle$. This yields $\langle j|\psi(t)\rangle = \frac{1}{n}\sum_{k=0}^{n-1} e^{-it\lambda_k}\omega^{jk}$. Thus,

$$p_j(t) = \frac{1}{n^2}\sum_{k,\ell} e^{-it(\lambda_k-\lambda_\ell)}\omega^{j(k-\ell)} = \frac{1}{n} + \frac{1}{n^2}\sum_{k\neq\ell} e^{-it(\lambda_k-\lambda_\ell)}\omega^{j(k-\ell)}. \tag{4}$$

Using the above, the average (limiting) probabilities are

$$\left|p_j - \frac{1}{n}\right| \ \le\ \frac{1}{n^2}\sum_{\lambda\in Sp(A)} \binom{m(\lambda)}{2} \ \le\ \frac{1}{n}\binom{\mu(G)}{2}. \tag{5}$$

So, if $\mu(G) = O(1)$, we have uniform mixing. □

*A graph is vertex-transitive if any pair of vertices has an automorphism mapping one vertex to the other.

Fig. 2. Some circulants with bounded eigenvalue multiplicity. From left to right: (i) the wheel V_8: a cycle plus a perfect matching. (ii) a double-loop circulant $\langle \pm 1, \pm 2 \rangle$ of order 7.

Theorem 2 *The continuous-time quantum walk on a constant-degree n-vertex circulant of the form $\langle 1, n/k_1, \ldots, n/k_d \rangle$, where, for each $j = 1, \ldots, d$, k_j is a constant which divides n, is average uniform mixing.*

Proof The eigenvalues of G are given by

$$\lambda_j = 2\cos\left(\frac{2\pi j}{n}\right) + 2\sum_{\ell=1}^{d} \cos\left(\frac{2\pi j}{k_\ell}\right), \tag{6}$$

for $j = 1, \ldots, n-1$. Since the sum $\sum_{\ell=1}^{d} \cos(2\pi j/k_\ell)$ can have at most $\prod_{\ell=1}^{d} k_\ell = O(1)$ distinct values, each eigenvalue must have a constant multiplicity. By Theorem 1, we have the claimed result. □

Corollary 1 *The continuous-time quantum walk on the 3-regular circulant "wheel" $V_n = \langle 1, n/2 \rangle$ of even order n is uniform mixing.*

4. Mixing on Join Bunkbeds

In this section, we study a circulant bunkbed structure obtained by the join of circulants. It is easy to see that the join $G + H$ of graphs G and H is obtained by connecting each vertex of G to each vertex of H, while maintaining the internal structures of G and H. For a graph G, the *cone* of G will denote the graph $K_1 + G$.

Lemma 1 *Let G and H be circulants of degrees k and ℓ, respectively. Suppose that the eigenvalues of G and H are $k = \mu_0 > \mu_1 \geq \ldots \geq \mu_{|G|-1}$ and $\ell = \nu_0 > \nu_1 \geq \ldots \geq \nu_{|H|-1}$, respectively. Then, the eigenvalues and (orthonormal) eigenvectors of $G + H$ are found in three separate sets $\{\langle \mu_a, |z_a^G\rangle\rangle \ : \ 1 \leq a \leq |G| - 1\}$, $\{\langle \nu_b, |z_b^H\rangle\rangle \ : \ 1 \leq b \leq |H| - 1\}$, and $\{\langle \lambda_\pm, |z_\pm\rangle\rangle\}$, where, for $x = 0, \ldots, |G||H| - 1$, we have*

$$\langle x|z_a^G\rangle = \frac{1}{\sqrt{|G|}}\, \omega_{|G|}^{ax}\, [\![x \in G]\!], \quad a = 1, \ldots, |G| - 1 \tag{7}$$

$$\langle x|z_b^H\rangle = \frac{1}{\sqrt{|H|}}\, \omega_{|H|}^{bx}\, [\![x \in H]\!], \quad b = 1, \ldots, |H| - 1 \tag{8}$$

$$\langle x|z_\pm\rangle = \frac{1}{L_\pm}\, (\beta_\pm)^{[\![x \in H]\!]}, \tag{9}$$

where $\beta_{\pm} = (\lambda_{\pm} - k)/|H|$, $L_{\pm} = \sqrt{|G| + |H|\beta_{\pm}^2}$, *and* $\lambda_{\pm}$ *are the roots of* $\lambda^2 - (k+\ell)\lambda - (|G||H| - k\ell) = 0$.

Proof Note that the adjacency matrix of $G + H$ is given by

$$A = \begin{bmatrix} A_G & J_{|G|\times|H|} \\ J_{|H|\times|G|} & A_H \end{bmatrix} \tag{10}$$

where $J_{p\times q}$ is the all-one matrix of dimension $p \times q$. It is easy to see that $|z_a^G\rangle$ are eigenvectors of A with eigenvalues μ_a, for $a = 1, \ldots, |G|-1$, and $|z_b^H\rangle$ are eigenvectors of A with eigenvalues ν_b, for $b = 1, \ldots, |H| - 1$. The last two eigenvectors are obtained by noting that the eigenvectors have the form $\begin{bmatrix} a & \ldots & a & b & \ldots & b \end{bmatrix}^T$. This gives the equations $ka + b|H| = \lambda a$ and $\ell b + a|G| = \lambda b$, whose solutions yield the eigenvalues $\lambda_{\pm} = \frac{1}{2}((k+\ell)^2 \pm \sqrt{\Delta})$, where $\Delta = (k-\ell)^2 + 4|G||H|$, and eigenvectors with $a = 1$ and $b = (\lambda_{\pm} - k)/|H|$. □

Theorem 3 *Suppose that* G *and* H *are circulants of degrees* k *and* ℓ*, respectively. Let* $\Delta = (k-\ell)^2 + 4|G||H|$ *and* $\lambda_{\pm} = 1/2[(k+\ell)^2 \pm \sqrt{\Delta}]$. *Consider a continuous-time quantum walk on* $G + H$ *starting at some vertex of* G. *Let* $\overline{p}_x(G)$ *denote the limiting probability of* $x \in G$ *over the subgraph* G. *Assume that*

$$\lambda_- \notin (Sp(G) \setminus \{k\}) \cup (Sp(H) \setminus \{\ell\}). \tag{11}$$

Then, the limiting probabilities of the vertices of $G + H$ *are*

$$\overline{p}_x(G+H) \;=\; \left\{ \left(\overline{p}_x(G) - \frac{1}{|G|} \right) + \frac{1}{|G|} \left(\frac{1}{|G|} - \frac{2|H|}{\Delta} \right) \right\} [\![x \in G]\!] \;+\; \frac{2}{\Delta} [\![x \in H]\!] \tag{12}$$

Proof Let the initial state be $|\psi(0)\rangle = |0\rangle$ where the quantum walk starts at a vertex of G. By Lemma 1, we have

$$|\psi(0)\rangle = \frac{1}{\sqrt{|G|}} \sum_{a=1}^{|G|-1} |z_a^G\rangle + \sum_{\pm} \frac{1}{L_{\pm}} |z_{\pm}\rangle, \tag{13}$$

and, thus,

$$|\psi(t)\rangle = \frac{1}{\sqrt{|G|}} \sum_{a=1}^{|G|-1} e^{-it\mu_a} |z_a^G\rangle + \sum_{\pm} \frac{e^{-it\lambda_{\pm}}}{L_{\pm}} |z_{\pm}\rangle. \tag{14}$$

The amplitude on vertex x at time t is given by

$$\langle x|\psi(t)\rangle = \frac{1}{|G|} \sum_{a=1}^{|G|-1} e^{-it\mu_a} \omega_{|G|}^{ax} + \sum_{\pm} \frac{e^{-it\lambda_{\pm}}}{L_{\pm}^2} \beta_{\pm}^{[\![x\in H]\!]}, \tag{15}$$

where $\beta_{\pm} = (\lambda_{\pm} - k)/|H|$, and we obtain

$$\overline{p}_x = \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathsf{d}t \; |\langle x|\psi(t)\rangle|^2 = \overline{p}_x(G) - \frac{1}{|G|} + \sum_{\pm} \left(\frac{\beta_{\pm}^{[\![x\in H]\!]}}{L_{\pm}^2} \right)^2, \tag{16}$$

where $\overline{p}_x(G)$ is the limiting probability on the subgraph G. After some calculations, we get

$$\sum_{\pm}\left(\frac{1}{L_{\pm}^2}\right)^2 = \frac{1}{|G|}\left(\frac{1}{|G|} - \frac{2|H|}{\Delta}\right), \quad \sum_{\pm}\left(\frac{\beta_{\pm}}{L_{\pm}^2}\right)^2 = \frac{2}{\Delta}, \tag{17}$$

which completes the stated claim. □

The single theorem above implies the following various known and new facts about mixing on the family of complete and related graphs. First, we obtain a perfect uniform mixing behavior on K_2, but not on K_n, for $n > 2$.

Corollary 2 *The continuous-time quantum walk on K_2 is average exactly uniform mixing.*

Proof By Theorem 3, we have $|G| = |H| = 1$ and $k = \ell = 0$. Thus, $\Delta = 4$, and therefore, $\overline{p}_0 = \overline{p}_1 = 1/2$. □

Corollary 3 *[2] The continuous-time quantum walk on K_n is not average uniform mixing, as $n \to \infty$.*

Proof By Theorem 3, we have $K_n = K_1 + K_{n-1}$. We have $|G| = 1$, $|H| = n-1$, $k = 0$, and $\ell = n-1$. Then, $\Delta = (n-1)^2 + 4n$, with $\overline{p}_0 = 1 - 2n/\Delta \sim 1$ and $\overline{p}_j = 2/\Delta \sim 0$, as $n \to \infty$. □

Next, we consider the cone of circulants. The following corollary provides a simple explanation why K_n is not average uniform mixing, for large n; it is because K_n is a cone of a dense circulant.

Corollary 4 *The continuous-time quantum walk on the cone of any circulant C, namely, $K_1 + C$, is not average uniform mixing.*

Proof Let C be a ℓ-regular circulant of order n. By Theorem 3, we have $|G| = 1$, $|H| = n$, $k = 0$. Then, $\overline{p}_0 = 1 - (1/2)[1/(1 + (\ell/2)^2/n)]$. Thus, $\overline{p}_0 = \Omega(1)$, regardless of ℓ. □

Homogeneous Joins of Circulants Consider the unbounded m-fold homogeneous join of a circulant G, namely, $G^{(+m)} = G + \ldots + G$, where there are m terms in the summation. The following theorem shows that the uniform mixing property of G transfers into its unbounded homogeneous join if m is a constant.

Theorem 4 *Let G be a circulant of order n. Let $m \geq 2$ is a constant and $n > 2\lambda_0(G)$. In the continuous-time quantum walk, $G^{(+m)} = \sum_{\ell=1}^{m} G$ is average uniform mixing if G is.*

Proof The adjacency matrix of $G^{(+m)} = \sum_{\ell=1}^{m} G$ is given by

$$A = I_m \otimes G + K_m \otimes J_n, \tag{18}$$

where I_m is the $m \times m$ identity matrix, K_m is a complete graph on m vertices, and J_n is the $n \times n$ all-one matrix. Since G is a circulant, both summands share the same set of the following orthonormal eigenvectors

$$\left\{|F_{j,k}\rangle = |F_j^{(m)}\rangle \otimes |F_k^{(n)}\rangle \ : \ 0 \le j \le m-1, 0 \le k \le n-1\right\}, \tag{19}$$

where $|F_j^{(m)}\rangle$ denotes the j-th column of the $m \times m$ Fourier matrix, and similary for $|F_k^{(n)}\rangle$. Let $\lambda_k(G)$, for $0 \le k \le n-1$, be the eigenvalues of G in descending order. The corresponding eigenvalues of $G^{(+m)}$ are given by

$$\lambda_{j,k} = \begin{cases} \lambda_0(G) + (m-1)n & \text{if } j = k = 0 \\ \lambda_0(G) - n & \text{if } j \neq 0 \text{ and } k = 0 \\ \lambda_k(G) & \text{if } j, k \neq 0 \end{cases} \tag{20}$$

If $|\psi(0)\rangle = |0\rangle \otimes |0\rangle$ then $|\psi(0)\rangle = 1/\sqrt{mn}\sum_{j=0}^{m-1}\sum_{k=0}^{n-1}|F_{j,k}\rangle$. Thus,

$$|\psi(t)\rangle = \frac{1}{\sqrt{mn}} \sum_{j=0}^{m} \sum_{k=0}^{n-1} e^{-it\lambda_{j,k}} |F_{j,k}\rangle. \tag{21}$$

Thus, for $x \in \mathbb{Z}_m$ and $y \in \mathbb{Z}_n$, we have

$$\psi_{x,y}(t) = \langle x, y|\psi(t)\rangle = \frac{1}{mn} \sum_{j=0}^{m} \sum_{k=0}^{n-1} e^{-it\lambda_{j,k}} \exp\left(\frac{2\pi ijx}{m}\right) \exp\left(\frac{2\pi iky}{n}\right). \tag{22}$$

Note that the three types of eigenvalues of $G^{(+m)}$ are mutually distinct, since

$$\lambda_0(G) - n \ < \ \lambda_k(G) \ < \ \lambda_0(G) + (m-1)n. \tag{23}$$

Therefore, we have

$$\left|\overline{p}_{x,y} - \frac{1}{mn}\right| \le \frac{1}{(mn)^2} \binom{m-1}{2} \left[1 + n\binom{\mu(G)}{2}\right] = O\left(\frac{\mu^2(G)}{mn}\right), \tag{24}$$

since m is a constant. □

The above theorem also *explains* why the complete graph K_N is not uniform mixing, since K_N can be viewed as a homogeneous m-fold join of $K_{N/m}$, for some constant m that divides N. The theorem also implies the following claim about the multipartite complete graphs.

Corollary 5 *The continuous-time quantum walk on the complete multipartite graph $K_n^{(m)}$ is not average uniform mixing if $m \ge 2$ is a constant.*

Proof Since a continuous-time quantum walk is not average uniform mixing on the empty graph $\overline{K}_n$ and $K_n^{(m)} = \overline{K}_n + \ldots + \overline{K}_n$, we have our claim. □

5. Mixing on Cartesian Bunkbeds

In this section, we consider a circulant bunkbed structure obtained by the Cartesian product $P_2 \times C$, where C is a circulant graph.

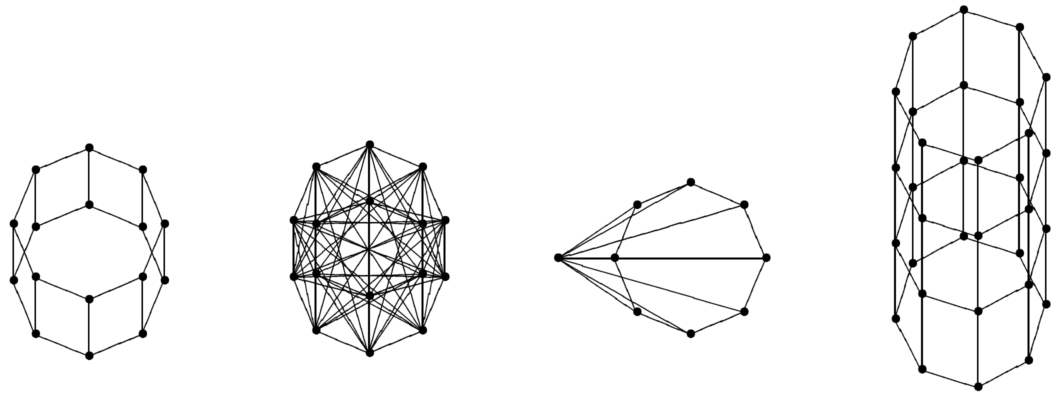

Fig. 3. Examples of circulant bunkbeds. (a) The double bunkbed: $P_2 \times C_8$. (b) The Join bunkbed: $C_8 + C_8$. (c) The Cone: $K_1 + C_8$. (d) The Cartesian bunkbed: $P_4 \times C_8$.

Lemma 2 *Let G be a circulant of degree d and order n, whose eigenvalues are $d = \mu_0 > \mu_1 \geq \ldots \geq \lambda_{n-1}$. Then, the eigenvalues of $P_2 \times G$ are $\lambda_j^{\pm} = \mu_j \pm 1$ with the following (orthonormal) set of eigenvectors*

$$|z_j^{\pm}\rangle = |\pm\rangle \otimes |z_j\rangle, \tag{25}$$

where $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$ and $\langle x|z_j\rangle = (1/\sqrt{|G|})\omega^{jx}$, for $j, x \in [n]$, with $\omega = e^{2\pi i/n}$.

Proof Note that the adjacency matrix of $P_2 \times G$ is given by $P_2 \otimes I_n + I_2 \otimes A_G$. Since P_2 is a circulant, both $P_2 \otimes I_n$ and $I_2 \otimes A_G$ are simultaneously diagonalizable by $|z_j^{\pm}\rangle$. This implies the stated claim on the spectra of $P_2 \times G$. □

Theorem 5 *Let G be a circulant of order n. In the continuous-time quantum walk, $P_2 \times G$ is average uniform mixing if G is.*

Proof Assume that $|\psi(0)\rangle = |0\rangle \otimes |0\rangle$. Thus, $|\psi(0)\rangle = \sum_{\pm} \frac{1}{\sqrt{2}}|\pm\rangle \otimes \sum_j \frac{1}{\sqrt{n}}|z_j\rangle$, and

$$|\psi(t)\rangle = e^{-itA}|\psi(0)\rangle = \frac{1}{\sqrt{2n}} \sum_{\pm,j} e^{-it\lambda_j^{\pm}} |\pm\rangle \otimes |z_j\rangle. \tag{26}$$

This implies that

$$\langle b, x|\psi(t)\rangle = \frac{1}{\sqrt{2n}} \sum_{\pm,j} e^{-it(\lambda_j \pm 1)} \langle b|\pm\rangle\langle x|z_j\rangle \tag{27}$$

$$= \frac{1}{2n} \sum_{\pm,j} e^{-it(\lambda_j \pm 1)} (\pm 1)^b \omega^{jx} \tag{28}$$

$$= \frac{1}{n} \sum_j e^{-it\lambda_j} \omega^{jx} \sum_{\pm} e^{-it(\pm 1)} (\pm 1)^b \tag{29}$$

$$= \frac{1}{n} \sum_j e^{-it\lambda_j} \omega^{jx} [(1-b)\cos(t) + b(-i\sin(t))] \tag{30}$$

Let $p_{b,x}(t) = |\langle b, x|\psi(t)\rangle|^2$. Thus,

$$p_{b,x}(t) = \frac{1}{n^2}\sum_{j,k}[(1-b)\cos^2(t) + b\sin^2(t)]e^{-it(\lambda_j-\lambda_k)}\omega^{(j-k)x}. \tag{31}$$

Note that $p_{0,x}(t) + p_{1,x}(t) = p_x(t)$, where $p_x(t)$ is the (instantaneous) probability on vertex x at time t of a quantum walk on G alone. Then,

$$\overline{p}_{0,x} = \frac{1}{n^2}\sum_{j,k}\omega^{(j-k)x}\lim_{T\to\infty}\frac{1}{T}\int_0^T \cos^2(t)e^{-it(\lambda_j-\lambda_k)}\ \mathsf{d}t = \frac{1}{2}\ \overline{p}_x, \tag{32}$$

since $\lim_{T\to\infty}\frac{1}{T}\int_0^T \cos^2(t)e^{-it\Delta}\ \mathsf{d}t = \frac{1}{2}\ [\![\Delta = 0]\!]$. Similarly, we obtain $\overline{p}_{1,x} = \frac{1}{2}\overline{p}_x$. This yields the claim. □

Corollary 6 *The continuous-time quantum walk on a Cartesian bunkbed $P_2 \times G$, where G is a d-degree circulant of the form $\langle 1, n/k_1, \ldots, n/k_{d-1}\rangle$, where d and $k_1, \ldots, k_{d-1}$ are constants, is average uniform mixing.*

Circulant Cylinders To extend our Cartesian bunkbeds over paths with more than two vertices, we provide, for completeness, an analysis of the quantum walk on paths. This problem is well-known in the physics literature, but is normally done on the infinite paths using different techniques [10]. The eigenvalues λ_j and eigenvectors $|Q_j\rangle$ of the path P_m (see [18]), for $j = 1, \ldots, m$, are defined as

$$\lambda_j = 2\cos\left(\frac{j\pi}{m+1}\right) \tag{33}$$

$$\langle x|Q_j\rangle = \frac{1}{\sqrt{(m+1)/2}}\ \sin\left(\frac{jx\pi}{m+1}\right), \quad x = 1, \ldots, m \tag{34}$$

If the quantum walk starts with the initial state $|\psi(0)\rangle = |1\rangle$, where the basis states are $|1\rangle, \ldots, |m\rangle$, then

$$|\psi(t)\rangle = \sum_{j=1}^{m}\frac{e^{-it\lambda_j}}{\sqrt{(m+1)/2}}\ \sin\left(\frac{j\pi}{m+1}\right)\ |Q_j\rangle. \tag{35}$$

Since P_m has m distinct eigenvalues, the limiting probabilities are given by

$$\overline{p}_x = \frac{4}{(m+1)^2}\sum_{j=1}^{m}\sin^2\left(\frac{j\pi}{m+1}\right)\sin^2\left(\frac{jx\pi}{m+1}\right). \tag{36}$$

Note that, since $\int_0^\pi \sin^2(t)\mathsf{d}t = \pi/2$, we get an upper bound of

$$\overline{p}_x \leq \frac{4}{(m+1)^2}\sum_{j=1}^{m}\sin^2\left(\frac{j\pi}{m+1}\right) \tag{37}$$

$$\leq \frac{4}{(m+1)\pi}\left(\int_0^\pi \sin^2(t)\ \mathsf{d}t\ +\ \frac{\pi}{(m+1)}\right) \tag{38}$$

$$\leq \frac{2}{(m+1)} + \frac{4}{(m+1)^2} = O\left(\frac{1}{m}\right), \tag{39}$$

which implies that the quantum walk on P_m is average uniform mixing.

The eigenvalues of a circulant cylinder $T = P_m \times G$, where G is a circulant of order n, are given by

$$\lambda_{j,k} = \mu_j + \nu_k, \qquad \text{where} \quad 1 \leq j \leq m, \quad 0 \leq k \leq n-1, \tag{40}$$

where $\mu_j = 2\cos(j\pi/(m+1))$ and ν_k are the eigenvalues of P_m and G, respectively. Since the adjacency matrix of T is defined as $P_m \otimes I_n + I_m \otimes G$, the eigenvectors of T are

$$|T_{j,k}\rangle = |Q_j\rangle \otimes |F_k\rangle, \qquad \text{where} \quad 1 \leq j \leq m, \quad 0 \leq k \leq n-1, \tag{41}$$

where $|Q_j\rangle$ and $|F_j\rangle$ are the eigenvectors of P_m and the circulant G, respectively. Recall that $\langle x|Q_j\rangle = \sqrt{\frac{2}{m+1}} \sin\left(\frac{jx\pi}{m+1}\right)$, for $1 \leq j, x \leq m$, and $\langle y|F_k\rangle = \frac{1}{\sqrt{n}} \exp\left(\frac{2\pi iky}{n}\right)$, for $0 \leq k, y \leq n-1$.

If the initial state is $|\psi(0)\rangle = |1\rangle \otimes |0\rangle$, we have

$$|\psi(0)\rangle = \sum_{j=1}^{m} \langle Q_j|1\rangle |Q_j\rangle \otimes \sum_{k=0}^{n-1} \langle F_k|0\rangle |F_k\rangle. \tag{42}$$

The adjacency matrix of $P_m \times G$ is given by $A = P_m \otimes I_n + I_m \otimes G$, where the two summands commute with each other. Thus, $e^{-itA} = e^{-it(P_m \otimes I_n)} e^{-it(I_m \otimes G)}$, and

$$|\psi(t)\rangle = \sum_{j=1}^{m} \langle Q_j|1\rangle e^{-it\mu_j} |Q_j\rangle \otimes \sum_{k=0}^{n-1} \langle F_k|0\rangle e^{-it\nu_k} |F_k\rangle. \tag{43}$$

The amplitudes of $|\psi(t)\rangle$ at vertex x on the path P_m and vertex y within the circulant G is given by

$$\langle x, y|\psi(t)\rangle \quad = \quad \sum_{j=1}^{m} e^{-it\mu_j} \langle x|Q_j\rangle \langle Q_j|1\rangle \sum_{k=0}^{n-1} e^{-it\nu_k} \langle y|F_k\rangle \langle F_k|0\rangle \tag{44}$$

Corollary 7 *Let G be a Cartesian product $P_m \times C$, where C is a circulant of order n. The continuous-time quantum walk on G is uniform mixing if m is constant or n is constant.*

6. Conclusions

It was known that a continuous-time quantum walk is uniform average mixing on the cycles C_n, but is not uniform average mixing on the complete graphs K_n and on the hypercubes Q_n. Our goal in this work was to provide a graph-theoretic explanation for this polarized phenomena.

First, we extend the phenomenon of the cycles, by showing that uniform mixing is achieved on circulants with bounded eigenvalue multiplicity. We also gave other explicit examples of circulants meeting this criteria. Second, we consider two graph-theoretic bunkbed structures over circulants in order to study the non-uniform mixing on K_n and Q_n. Our analysis on the join bunkbed sheds some light on the non-uniform mixing of the complete multipartite graphs (which includes K_n). Our analysis of the Cartesian bunkbed of circulants highlights a difference between the $\mathbb{Z}_n$-circulants and the $(\mathbb{Z}_2)^n$-circulants (see [8]). We leave a similar investigation of general group-theoretic circulants and Cayley graphs for future work (see [11]).

Acknowledgments

This research was supported by the National Science Foundation grant DMS-0353050 while the authors were part of the Clarkson-Potsdam Research Experience for Undergraduates (REU) Summer program in Mathematics at State University of New York at Postdam. The research of C. Tamon was also supported by the National Science Foundation grant DMR-0121146 through the Center for Quantum Device Technology at Clarkson University.

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