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# UNIVERSAL MIXING OF QUANTUM WALK ON GRAPHS

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We study the set of probability distributions visited by a continuous-time quantum walk on graphs. An edge-weighted graph $G$ is *universal mixing* if the instantaneous or average probability distribution of the quantum walk on $G$ ranges over all probability distributions on the vertices as the weights are varied over non-negative reals. The graph is *uniform* mixing if it visits the uniform distribution. Our results include the following:

- All weighted complete multipartite graphs are instantaneous universal mixing. This is in contrast to the fact that no *unweighted* complete multipartite graphs are uniform mixing (except for the four-cycle $K_{2,2}$).
- For all $n \geq 1$, the weighted claw $K_{1,n}$ is a minimally connected instantaneous universal mixing graph. In fact, as a corollary, the unweighted $K_{1,n}$ is instantaneous uniform mixing. This adds a new family of uniform mixing graphs to a list that so far contains only the hypercubes.
- Any weighted graph is average almost-uniform mixing unless its spectral type is sublinear in the size of the graph. This provides a nearly tight characterization for average uniform mixing on circulant graphs.
- No weighted graphs are average universal mixing. This shows that weights do not help to achieve average universal mixing, unlike the instantaneous case.

Our proofs exploit the spectra of the underlying weighted graphs and path collapsing arguments.

*Keywords*: Quantum walks, continuous-time, universal mixing

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## 1. Introduction

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The theory of random walks on graphs is an important topic in mathematics, physics, and computer science [25, 6, 12]. In recent years, a generalization of the classical random walks – called quantum walks – has gained considerable interest in the quantum information and computation research areas due to its potential applications [1]. In particular, the study of continuous-time quantum walks on graphs has shown promising applications in the algorithmic and implementation aspects. As an alternate algorithmic technique to the Quantum Fourier Transform and the Amplitude Amplification techniques, Childs *et al.* [7] demonstrated the power of continuous-time quantum walk algorithm for solving a specific blackbox graph search problem. As a generalization of classical random walks, the dynamics of quantum walks reveal unique characteristics. Moore and Russell [24] proved faster mixing times of quantum walks on the hypercubes. Kendon and Tregenna [19, 21] observed a striking phenomena that decoherence can improve the mixing dynamics of discrete quantum walks. This observation was subsequently confirmed for continuous-time quantum walks in [4, 11].

In this paper, we study the set of probability distributions generated by continuous-time quantum walks on edge-weighted graphs. Previous works had studied the question of whether a quantum walk on certain graphs visits the uniform distribution on the vertices of the graph [24, 2, 14]. Here, we consider graphs which visit *all* probability distributions on the vertex set of the graph. We call such graphs having the *universal mixing* property, whereas graphs that hit the uniform distribution have the *uniform mixing* property. We consider both the *instantaneous* and *average* distributions for such quantum walks. It is necessary to allow symmetric edge-weights on our graphs, since no unweighted graphs are universal mixing (although some, like the hypercubes, are uniform mixing [24]).

Our study of universal mixing via quantum walks is motivated by recent works in random walks on graphs. In [20], Kindler and Romik provided a characterization of the set of distributions computable by random walks on finite state generators (directed graphs with outputs). In another set of works, Boyd *et al.* [8, 9] studied the problem of finding the set of edge weights on a fixed given graph so as to obtain the fastest mixing time for the random walk. In the context of these works, the main problem that we study is as follows: given a fixed family of graphs, as we vary the edge weights on these graphs, will the quantum walk visit all probability distributions on the vertices? Stated differently, we are looking for a set of edge weights that allows the quantum walk to hit any specified probability distribution. Our main goal in this work is to discover and characterize graphs which allow such *universal* mixing property, as well as the more restricted uniform mixing property.

First, we prove that complete multipartite graphs are instantaneous universal mixing. These are classes of graphs whose vertices are partitioned into disjoint sets, where all edges are present except for edges connecting vertices from the same partition. In contrast, it is known that none of the unweighted complete multipartite graphs are uniform mixing, except for the four-cycle $K_{2,2}$ (see [2]). To show our multipartite theorem, we prove that the weighted three-vertex path $P_3$ and the claw (star) graph $K_{1,n}$ are both instantaneous universal mixing (see Figure (1) for examples of both graphs). Our proofs employ a generalization of the *path collapsing* technique used in [7], adapted for weighted graphs. In [7], a path collapsing argument was used to show a fast hitting time of a continuous-time quantum walk on *glued tree* graphs; whereas, in this paper we use a generalization of the argument to show universal

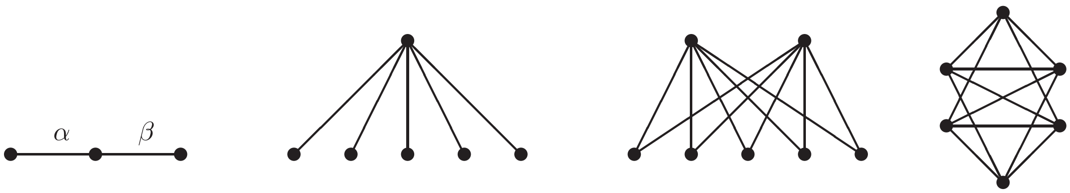



Fig. 1. Examples of edge-weighted graphs that are instantaneous universal mixing. From left to right: (a) path $P_3$; (b) claw $K_{1,5}$; (c) bipartite double-claw $K_{2,5}$; (d) 4-partite $K_{2,2,2,2}$.

mixing on multipartite graphs.

In fact, the claw is a minimally connected graph that is universal mixing, since it forms a tree on the set of vertices. This shows that any graph with a claw subgraph is also instantaneous universal mixing. As a corollary, we observe that the *unweighted* claws are instantaneous uniform mixing. This adds a new family of uniform mixing graphs to a list that so far contains only the hypercubes [24].

Next, we consider a *closure* result on graphs with instantaneous uniform mixing. More specifically, the Cartesian product $G \oplus H$ of two uniform mixing graphs $G$ and $H$ is also uniform mixing provided the two graphs share a common mixing time. This is the fundamental property used to show that the hypercubes $Q_n$ are uniform mixing, since they are the $n$-fold Cartesian product of the complete 2-vertex graph $K_2$ with itself [24]. We obtain several other classes of graphs with uniform mixing by combining the hypercubes $Q_n$ and the claws $K_{1,n}$, for $n \geq 1$, the complete three-vertex and four vertex graphs ($K_3$ and $K_4$), using the Cartesian product operator. Since the three- and four-vertex cycles are equivalent to $K_3$ and $Q_2$, respectively, they are also uniform mixing. The status of the $n$-cycles $C_n$ is still open though; but we show that $C_5$ is *not* uniform mixing.

Finally, we prove that no weighted graphs are average universal mixing. Intuitively, this is because the quantum walk never forgets its start vertex; or, more formally, the average probability weight of the start vertex is bounded away from zero. In the case of uniform mixing, we observe that a necessary condition for a weighted graph to be an average uniform mixing is for its spectral type (the number of distinct eigenvalues) to be linear in the size of the graph. This provides a nearly tight characterization for circulant graphs since these graphs are average almost-uniform mixing if their eigenvalues have bounded multiplicities [22].

In this paper, our focus is on continuous-time quantum walks. For a more complete exposition on quantum walks, the interested reader is referred to the excellent surveys by Kendon and Kempe [18, 19, 17].

## 2. Preliminaries

*Notation:* For a logical statement $S$, the Iversonian $[\![S]\!]$ (introduced in [13]) denotes the characteristic function of $S$ which evaluates to 1 if $S$ is true, and to 0 if it is false.

We consider graphs $G = (V, E)$ that are simple (no self-loops) and undirected, with edge weights. The edge weights are given by a non-negative real-valued function $\alpha : E \to \mathbb{R}^+ \cup \{0\}$

that is symmetric, i.e., $\alpha_{j,k} = \alpha_{k,j}$, for all $j, k \in V$. Let $A_G$ be the adjacency matrix of $G$, where $A_G[j,k] = \alpha_{j,k}[\![(j,k) \in E]\!]$. The set of eigenvalues of $A_G$ is denoted $Sp(G)$, and the (algebraic) multiplicity of an eigenvalue $\lambda$ 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 $G$. The maximum (algebraic) multiplicity of any eigenvalue of graph $G$ is denoted $\mu(G)$.

Some of the families of graphs studied here include paths $P_n$, cycles $C_n$, hypercubes $Q_n$, complete graphs $K_n$, complete multipartite graphs $K_n^{(k)}$, and circulant graphs. A complete multipartite graph $K_n^{(k)}$ is the graph complement of $k$ disjoint complete graphs $K_n$. A graph is a *circulant* graph if its adjacency matrix is a circulant matrix. A circulant matrix $A$ is completely 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 $n$. The Cartesian product of two graphs $G$ and $H$, denoted $G \oplus H$, is the graph defined on the vertex set $G \times H$, where $(g_1, h_1)$ is adjacent to $(g_2, h_2)$ if $g_1 = g_2$ and $(h_1, h_2) \in E(H)$; or $(g_1, g_2) \in E(G)$ and $h_1 = h_2$ (see page 617, [23]). Further background on graphs and their spectral properties are given in [6, 5].

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 [12, 10]). 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

$$|\psi(t)\rangle = e^{-itA_G}|\psi(0)\rangle, \tag{1}$$

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 $\langle x|\psi(0)\rangle = [\![x = \textsc{start}]\!]$, for some vertex $\textsc{start}$. The amplitude of the quantum walk of vertex $j$ at time $t$ is given by $\psi_j(t) = \langle j|\psi(t)\rangle$. The *instantaneous* probability of vertex $j$ at time $t$ is $p_j(t) = |\psi_j(t)|^2$. The *average* probability of vertex $j$ is defined as

$$\overline{p}_j = \lim_{T\to\infty} \frac{1}{T} \int_0^T p_j(t)\ \mathsf{d}t. \tag{2}$$

The average probability distribution of the quantum walk will be denoted $\overline{P}$. This notion of average distribution (defined in [1] for discrete-time quantum walks) is similar to the notion of a stationary distribution in classical random walks [3].

**Definition 1** *(Universal and Uniform Mixing)*
*Let $G = (V, E)$ be a simple, undirected, and connected graph that is edge-weighted. Then, $G$ has the instantaneous (or average)* universal mixing *property if for any probability distribution $D$ over the vertex set $V$ and for any start vertex $x$, there is a set of non-negative real weights on $E$, so that the continuous-time quantum walk on the weighted $G$, starting from $x$, has an instantaneous probability distribution at time $t$ (or average distribution) that equals $D$.*

*If the above condition holds for $D$ being the uniform distribution on $V$, we say $G$ has the instantaneous (or average)* uniform mixing *property. The mixing is* almost-uniform *if the instantaneous (or average) probability of each vertex is at most $O(1/|V|)$.*

**Example:** A quantum walk on the connected 2-vertex graph $K_2$ is given by

$$\exp\left\{-it\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right\}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}\cos(t)\\ -i\sin(t)\end{pmatrix}. \tag{3}$$

Thus, the instantaneous probability distribution of the quantum walk is $p(t) = [\cos^2(t)\ \sin^2(t)]^T$. This shows that the quantum walk on $K_2$ can generate *any* probability distribution on the two vertices. Unfortunately, this case does not generalize to arbitrarily many vertices. It was shown in [2] that the instantaneous probability distribution quantum walk on the complete graph $K_n$ *never* visits the uniform distribution on $n$ vertices, for any $n > 4$. A main question considered in this work is: will the quantum walk visit the uniform distribution if edge weights are allowed? In fact, as we vary the edge weights on $K_n$, will the quantum walk visit *all* probability distributions on $n$ elements (as is the case with the unweighted $K_2$)? We answer both questions in this paper; moreover, we will exhibit a family of minimally connected graphs with such universal property. Note that in a classical random walk, the interference phenomenon commonly observed in a quantum walk does not exist; thus, it is impossible for vertices reachable from the start vertex to have a zero probability.

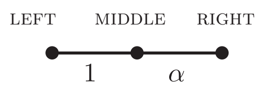
## 3. Instantaneous Universal Mixing

In this section, we prove that all weighted complete multipartite graphs are instantaneous universal mixing. First, we prove some results about the weighted 3-path $P_3$ and claw $K_{1,n}$.

**Lemma 1** *The weighted $P_3$ has instantaneous universal mixing.*

*Proof* Without loss of generality, we assume that the weights on $P_3$ are 1 and $\alpha$; since we can always scale the first weight to unity. Let $A$ be the adjacency matrix of $G$.

$P_3$ :




$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & \alpha \\ 0 & \alpha & 0 \end{pmatrix}$$

The eigenvalues of $A$ are $\lambda_0 = 0$ and $\lambda_\pm = \pm\Delta$, where $\Delta = \sqrt{1+\alpha^2}$, with the following set of orthonormal eigenvectors:

$$|v_0\rangle = \frac{1}{\Delta}\begin{pmatrix} -\alpha \\ 0 \\ 1 \end{pmatrix}, \qquad |v_\pm\rangle = \frac{1}{\sqrt{2\Delta^2}}\begin{pmatrix} 1 \\ \pm\Delta \\ \alpha \end{pmatrix}, \tag{4}$$

We have two cases to consider depending on the starting vertex of the quantum walk.

**case A:** The quantum walk starting at the left vertex is given by:

$$e^{-itA}|\text{LEFT}\rangle = \frac{-\alpha}{\Delta}|v_0\rangle + \frac{1}{\sqrt{2\Delta^2}}\sum_{\pm} e^{\mp it\Delta}|v_\pm\rangle = \frac{1}{\Delta^2}\begin{pmatrix} (\alpha^2 + \cos(\Delta t)) \\ -i\Delta\sin(\Delta t) \\ \alpha(\cos(\Delta t) - 1) \end{pmatrix} \tag{5}$$

Thus, the instantaneous probability distribution at time $t$ is:

$$p_{\text{LEFT}}(t) = (1-2\Gamma)^2, \quad p_{\text{MIDDLE}}(t) = 4\Gamma(1-\Gamma\Delta^2), \quad p_{\text{RIGHT}}(t) = \alpha^2(2\Gamma)^2, \tag{6}$$

where $\Gamma = \sin^2(\Delta t/2)/\Delta^2$. Combining the first and third expressions, we get $\alpha = \sqrt{p_{\text{RIGHT}}(t)}/(1-\sqrt{p_{\text{LEFT}}(t)})$, which shows that $(\alpha, t)$ can be selected to satisfy any probability distribution on the three vertices.

**case B:** The quantum walk starting at the middle vertex is given by:

$$e^{-itA}|\textsc{middle}\rangle = \frac{1}{\sqrt{2\Delta^2}} \sum_{\pm} (\pm\Delta) e^{\mp it\Delta} |v_\pm\rangle = \frac{1}{\Delta} \begin{pmatrix} -i\sin(\Delta t)) \\ \Delta\cos(\Delta t) \\ -i\alpha\sin(\Delta t) \end{pmatrix} \tag{7}$$

Thus, the instantaneous probability distribution at time $t$ is:

$$p_{\textsc{left}}(t) = \frac{\sin^2(\Delta t)}{\Delta^2}, \quad p_{\textsc{middle}}(t) = \cos^2(\Delta t), \quad p_{\textsc{right}}(t) = \alpha^2 \frac{\sin^2(\Delta t)}{\Delta^2}. \tag{8}$$

Thus $\alpha = \sqrt{p_{\textsc{right}}}/\sqrt{p_{\textsc{left}}}$, and hence, we see that $(\alpha, t)$ can be chosen to satisfy any required probability triples. □

In the following, we show that the weighted claw (star) graph is instantaneous universal mixing, for an arbitrary starting vertex. We will use Lemma 1 to prove this in combination with a weighted version of the *path collapsing* argument (used in [7]).

**Theorem 1** *The weighted $K_{1,n}$ has instantaneous universal mixing, for $n \geq 1$. Moreover, the weighted complete graphs $K_n$ are also instantaneous universal mixing, for $n \geq 1$.*

*Proof* Let the edge weights on the claw be $\alpha_1, \ldots, \alpha_n$, respectively. Then, the adjacency matrix is given by:

$$A = \begin{pmatrix} 0 & \alpha_1 & \alpha_2 & \ldots & \alpha_n \\ \alpha_1 & 0 & 0 & \ldots & 0 \\ \alpha_2 & 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \alpha_n & 0 & 0 & \ldots & 0 \end{pmatrix} \tag{9}$$

The eigenvalues of $A$ are $\lambda_\pm = \pm\Delta$, where $\Delta = \sqrt{\sum_{k=1}^n \alpha_k^2}$, and $\lambda_0 = 0$. The eigenvalues $\lambda_\pm$ are simple, whereas 0 has multiplicity $n-1$. The eigenvectors are given by:

$$|v_\pm\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \pm\alpha_1/\Delta & \ldots & \pm\alpha_n/\Delta \end{pmatrix}^T \tag{10}$$

$$|v_0\rangle = \begin{pmatrix} 0 & y_1 & \ldots & y_n \end{pmatrix}^T, \quad \text{where } \textstyle\sum_{k=1}^n \alpha_k y_k = 0 \tag{11}$$

Depending on whether the quantum walk starts at the center of the claw or not, we have two cases to analyze.

**case A:** The quantum walk starting at the center of the claw is given by:

$$|\psi(t)\rangle = e^{-itA} \sum_{\pm} \frac{1}{\sqrt{2}} |v_\pm\rangle \tag{12}$$

which yields $\langle\textsc{center}|\psi(t)\rangle = \cos(\Delta t)$, and $\langle k|\psi(t)\rangle = -i\alpha_k \sin(\Delta t)/\Delta$, for $k = 1, \ldots, n$. Thus, the instantaneous probabilities are given by:

$$p_{\textsc{center}}(t) = \cos^2(\Delta t), \quad p_k(t) = \frac{\alpha_k^2}{\Delta^2} \sin^2(\Delta t), \quad \text{where } k = 1, \ldots, n \tag{13}$$

This shows that the above instantaneous probabilities ranges over all probability distributions on $n+1$ vertices as $t$ and the $\alpha_k$'s range over $\mathbb{R}^+ \cup \{0\}$.

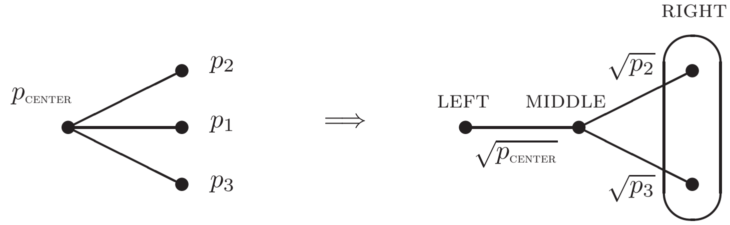



Fig. 2. Case B: the claw $K_{1,3}$ is universal mixing, when START $\neq$ CENTER; a reduction to $P_3$. The start vertex is labeled by $p_1$ and the target probabilities (left) are *shifted* onto the edges of the graph (right).

**case B:** We can assume without loss of generality that the quantum walk starts at vertex $k = 1$. But, this case is similar to the weighted $P_3$ case where vertex 1 is LEFT, the center of the claw is MIDDLE, and the rest of the other vertices are viewed as RIGHT; see Figure 2. A more formal argument for this reduction is as follows. Given the target probabilities $p_1$, $p_{\text{CENTER}}$, and $p_2, \ldots, p_n$, we define the weights on $K_{1,n}$ as follows: $w(1, \text{CENTER}) = \sqrt{p_{\text{CENTER}}}$ and $w(\text{CENTER}, k) = \alpha_k$, where $\alpha_k = \sqrt{p_k}$, for $k = 2, \ldots, n$. Along with the states $|\text{LEFT}\rangle = |1\rangle$ and $|\text{MIDDLE}\rangle = |\text{CENTER}\rangle$, we define a new state:

$$|\text{RIGHT}\rangle = \sum_{k=2}^{n} \frac{\alpha_k}{\widetilde{\Delta}} |k\rangle, \qquad \text{where } \widetilde{\Delta} = \sqrt{\textstyle\sum_{k=2}^{n} \alpha_k^2}. \tag{14}$$

Under this new reduced basis, the quantum walk on $K_{1,n}$, starting at vertex 1, is expressed using a *collapsed* Hamiltonian on $P_3$:

$$|\Psi(t)\rangle = \exp\left\{ -it \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & \widetilde{\Delta} \\ 0 & \widetilde{\Delta} & 0 \end{pmatrix} \right\} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \tag{15}$$

Note that the amplitudes $\langle k|\Psi(t)\rangle$ in the original $K_{1,n}$ is proportional to the amplitude $\langle \text{RIGHT}|\Psi(t)\rangle$, where the constant of proportionality is given by $\alpha_k$. Next, we find a mixing time $T$ on the weighted $P_3$ with the probabilities $p_{\text{LEFT}}(T) = p_1$, $p_{\text{MIDDLE}}(T) = p_{\text{CENTER}}$, and $p_{\text{RIGHT}}(T) = \sum_{k=2}^{n} p_k$. At time $T$, the probability of vertex $k$ in $K_{1,n}$ is $p_k(T) = \alpha_k^2/\Delta^2 \times p_{\text{RIGHT}}(T)$, which equals the target probability $p_k$, for all $k = 2, \ldots, n$. $\square$

For the next result, we generalize the previous theorem on $K_{1,n}$ to arbitrary complete multipartite graphs.

**Theorem 2** *All weighted complete bipartite graphs $K_{m,n}$ are instantaneous universal mixing, for all $m, n \geq 1$.*

*Proof* If $m = 1$, $K_{m,n}$ is universal mixing by Theorem 1. Now, assume that $m > 1$. Let $A = \{a_0, a_1, \ldots, a_m\}$ and $B = \{b_1, \ldots, b_n\}$ be the two partitions of the bipartite graph $G = K_{m+1,n}$, with $|A| = m + 1$ and $|B| = n$. Without loss of generality, let the start vertex

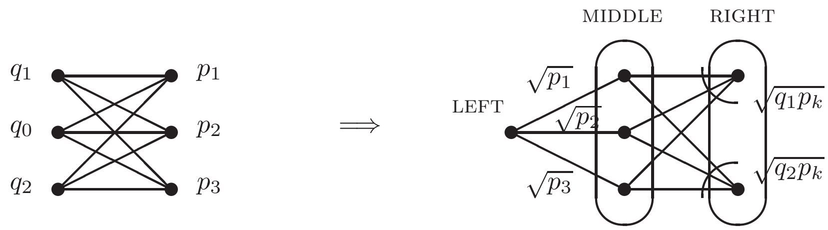



Fig. 3. The complete bipartite graph $K_{3,3}$ is universal mixing: by a reduction to $P_3$. The start vertex is labeled by $q_0$. The target probabilities $q_0, q_1, q_2$ and $p_1, p_2, p_3$ (left) are transferred onto the edge weights of the graph (right).

be $a_0$. Viewing the start vertex as its own partition, we have a weighted 3-path where $a_0$, $B$ and $C = A \setminus \{a_0\}$ form the *vertices* of $P_3$.

Let $p_1, \ldots, p_n$ be the required probabilities on the vertices of $B$ and let $q_1, \ldots, q_m$ be the required probabilities on the vertices of $C$. Let $\alpha_j = \sqrt{p_j}$, for $j = 1, \ldots, n$, and $\beta_k = \sqrt{q_k}$, for $k = 1, \ldots, m$, with $\Delta = \sqrt{\sum_{j=1}^n \alpha_j^2}$ and $\Gamma = \sqrt{\sum_{k=1}^m \beta_k^2}$. Now, we define the following edge weights on $G$:

$$w(a_0, b_j) = \alpha_j, \quad \text{where } j = 1, \ldots, n \tag{16}$$

$$w(b_j, a_k) = \alpha_j \beta_k, \quad \text{where } j = 1, \ldots, n \text{ and } k = 1, \ldots, m\ , \tag{17}$$

while the other weights are zero. Consider the following quantum states

$$|\text{LEFT}\rangle = |a_0\rangle, \quad |\text{MIDDLE}\rangle = \frac{1}{\Delta} \sum_{j=1}^{n} \alpha_j |a_j\rangle, \quad |\text{RIGHT}\rangle = \frac{1}{\Gamma} \sum_{k=1}^{m} \beta_k |b_k\rangle. \tag{18}$$

Under the basis states $\{|\text{LEFT}\rangle, |\text{MIDDLE}\rangle, |\text{RIGHT}\rangle\}$, we have the following *collapsed* Hamiltonian for a weighted $P_3$:

$$\mathbb{H} = \begin{pmatrix} 0 & \Delta & 0 \\ \Delta & 0 & \Delta\Gamma \\ 0 & \Delta\Gamma & 0 \end{pmatrix} \tag{19}$$

In the quantum walk $|\Psi(t)\rangle = \exp(-it\mathbb{H})|a_0\rangle$, note that the amplitude $\langle b_j|\Psi(t)\rangle$ in the original $K_{m,n}$ is proportional to the amplitude $\langle \text{MIDDLE}|\Psi(t)\rangle$ by the constant $\alpha_j$, whereas the amplitude $\langle a_k|\Psi(t)\rangle$ is proportional to the amplitude $\langle \text{RIGHT}|\Psi(t)\rangle$ by the constant $\beta_k$.

In the weighted $P_3$, we find a mixing time $T$ for which $p_{\text{MIDDLE}}(T) = \sum_{j=1}^n p_j$ and $p_{\text{RIGHT}}(T) = \sum_{k=1}^m q_k$. At this time $T$, the probability of vertex $b_j$ is given by $\alpha_j^2/\Delta^2 \times p_{\text{MIDDLE}}(T) = p_j$, and the probability of vertex $a_k$ is given by $\beta_k^2/\Gamma^2 \times p_{\text{RIGHT}}(T) = q_k$. This completes the claim. □

**Theorem 3** *All weighted complete $k$-partite graphs are instantaneous universal mixing, for $k \geq 2$.*

*Proof* We prove the claim by induction on $k$. For $k = 2$, we have a complete bipartite graph which is universal mixing by Theorem 2. Assuming the claim is true for all $k < \ell$, any complete $\ell$-partite graph contains a complete $(\ell - 1)$-partite subgraph (by disconnecting two arbitrary partitions), and thus, it is universal mixing. This proves the claim. □

The above theorem stands in contrast to the fact that (unweighted) complete multipartites, with the exception of $K_{2,2}$, are not instantaneous uniform mixing (see [2]).

## 4. Instantaneous Uniform Mixing

The only unweighted graphs known to be uniform mixing are the hypercubes $Q_n$ [24] and the two complete graphs, $K_3$ and $K_4$ [2]. To this small list, we add another family of graphs.

**Corollary 1** *The family of (unweighted) claw $K_{1,n}$ graphs is instantaneous uniform mixing.*

*Proof* Apply Theorem 1 with $\alpha_k = 1$, $k = 1, \ldots, n$, and $t = \cos^{-1}(1/\sqrt{n+1})/\sqrt{n}$. □

In what follows, we state a *closure* result for graphs that are uniform mixing.

**Fact 4** *If $G, H$ are graphs with instantaneous uniform mixing, then so is $G \oplus H$, assuming that their mixing times have a common intersection.*

*Proof* Let $\{\langle \mu_j, |v_j\rangle\rangle\}_j$ and $\{\langle \nu_k, |w_k\rangle\rangle\}_k$ be the spectra of $G$ and $H$, respectively. The adjacency matrix of $G \oplus H$ is given by $I \otimes G + H \otimes I$, which is a sum of two commuting matrices. Hence, $|v_j\rangle \otimes |w_k\rangle$ are the eigenvectors of $G \oplus H$ with eigenvalues $\mu_j + \nu_k$, for all $j, k$. Without loss of generality, assume that the start vertex is $|0\rangle_G \otimes |0\rangle_H$. Also, suppose that $|0\rangle_G = \sum_j \alpha_j |v_j\rangle$ and $|0\rangle_H = \sum_k \beta_k |w_k\rangle$ are the initial states in $G$ and $H$, respectively. Then, the quantum walk on $G \oplus H$ is given by

$$\sum_{j,k} (\alpha_j e^{-it\mu_j} |v_j\rangle) \otimes (\beta_k e^{-it\nu_k} |w_k\rangle) = e^{-itG} |0\rangle_G \otimes e^{-itH} |0\rangle_H \tag{20}$$

This shows that if the mixing times of $G$ and $H$ have a common intersection, then $G \oplus H$ is instantaneous uniform mixing. □

**Proposition 5** *The following graphs are instantaneous uniform mixing:*

*(a) $G^{\oplus k}$, $k \geq 1$, if the weighted graph $G$ is instantaneous uniform mixing.*

*(b) Any Cartesian product combinations of $Q_n$ and $K_4$, for any $n \geq 1$.*

*Proof* (a) Apply Fact 4 to $G$ with itself recursively $n - 1$ times. (b) It was shown in [24], the hypercube $Q_n$ hits the uniform distribution at times $t = (2k + 1)n\pi/4$. For the complete

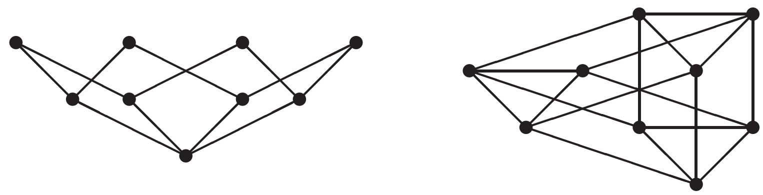


Fig. 4. Examples of instantaneous uniform mixing graphs: from left to right: (a) $P_3 \oplus P_3$; (b) $K_3 \oplus K_3$.

graphs $K_n$, it was proved in [2] that uniform mixing is possible if and only if

$$\frac{4}{n}\sin^2\left(\frac{tn}{2(n-1)}\right) = 1. \tag{21}$$

So, for $K_3$, uniform mixing is achieved if $\sin^2(3t/4) = 3/4$ (or $3t/4 = \sin^{-1}(\pm\sqrt{3}/2)$), and for $K_4$, if $\sin^2(2t/3) = 1$ (or $t = (2k+1)(3\pi/4)$). Note that the uniform mixing times of $Q_n$ and $K_4$ have common intersections. □

It is not known if the cycles $C_n$, weighted or not, are uniform mixing [2], except for $C_3 = K_3$ and $C_4 = Q_2$. In the following, we show that $C_5$ is not uniform mixing.

**Fact 6** *The unweighted $C_5$ is not instantaneous uniform mixing.*

*Proof* The eigenvalues of $C_5$ are $\lambda_j = 2\cos(2\pi j/5)$, $j = 0, \ldots, 4$ (see [5]). In fact, they exhibit some symmetries since $\lambda_0 = 2$, $\lambda_1 = \lambda_4 = 2\cos\left(\frac{2\pi}{5}\right) = (-1+\sqrt{5})/2$, and $\lambda_2 = \lambda_3 = 2\cos\left(\frac{4\pi}{5}\right) = (-1-\sqrt{5})/2$. Let $\lambda_\pm = (-1 \pm \sqrt{5})/2$; thus, $\lambda_1 = \lambda_+$ and $\lambda_2 = \lambda_-$.

The eigenvectors of $C_5$ are $|v_j\rangle$, where $\langle k|v_j\rangle = \omega^{jk}/\sqrt{5}$, for $j, k = 0, \ldots, 4$ and $\omega = \exp(2\pi i/5)$. Given that $|0\rangle = \frac{1}{\sqrt{5}}\sum_{j=0}^{4}|v_j\rangle$, the quantum walk on $C_5$ is given by:

$$|\psi(t)\rangle = \frac{1}{\sqrt{5}}\left\{e^{-2it}|v_0\rangle + e^{-it\lambda_1}(|v_1\rangle + |v_4\rangle) + e^{-it\lambda_2}(|v_2\rangle + |v_3\rangle)\right\}. \tag{22}$$

We note that $|v_1\rangle + |v_4\rangle = \frac{1}{\sqrt{5}}[\lambda_0\lambda_+\lambda_-\lambda_-\lambda_+]^T$ and $|v_2\rangle + |v_3\rangle = \frac{1}{\sqrt{5}}[\lambda_0\lambda_-\lambda_+\lambda_+\lambda_-]^T$. Thus, the amplitude of the quantum walk is given by

$$\langle 0|\psi(t)\rangle = \frac{1}{5}\left\{e^{-it\lambda_0} + \sum_{\pm}\lambda_0 e^{-it\lambda_\pm}\right\} \tag{23}$$

$$\langle 1|\psi(t)\rangle = \langle 4|\psi(t)\rangle = \frac{1}{5}\left\{e^{-it\lambda_0} + \sum_{\pm}\lambda_\pm e^{-it\lambda_\pm}\right\} \tag{24}$$

$$\langle 2|\psi(t)\rangle = \langle 3|\psi(t)\rangle = \frac{1}{5}\left\{e^{-it\lambda_0} + \sum_{\pm}\lambda_\mp e^{-it\lambda_\pm}\right\} \tag{25}$$

Let $\mu_\pm = (5 \pm \sqrt{5})/2$. After simplifications, the probability function is given by:

$$p_0(t) = \frac{1}{25}\left\{9 + 4\sum_{\pm}\cos(\mu_\pm t) + 8\cos(\sqrt{5}t)\right\} \tag{26}$$

$$p_1(t) = p_4(t) = \frac{1}{25}\left\{4 + \sum_{\pm} 2\lambda_\mp \cos(\mu_\pm t) - 2\cos(\sqrt{5}t)\right\} \tag{27}$$

$$p_2(t) = p_3(t) = \frac{1}{25}\left\{4 + \sum_{\pm} 2\lambda_\pm \cos(\mu_\pm t) - 2\cos(\sqrt{5}t)\right\} \tag{28}$$

Assume that $C_5$ has instantaneous uniform mixing at time $T$. From $p_1(T) = p_2(T)$, we get $\cos(\mu_+ T) = \cos(\mu_- T)$ which implies that $\mu_+ = 2\pi m \pm \mu_-$, for some $m \in \mathbb{Z}$. So, we get either $\sqrt{5}T = 2\pi m$ or $5T = 2\pi m$. From $p_0(T) = p_2(T)$, we get

$$5 + (5+\sqrt{5})\cos(\mu_- T) + (5-\sqrt{5})\cos(\mu_+ T) + 10\cos(\sqrt{5}T) = 0. \tag{29}$$

If $\sqrt{5}T = 2\pi m$, then $(5+\sqrt{5})\cos(\mu_- T) + (5-\sqrt{5})\cos(\mu_+ T) + 15 = 0$, which is a contradiction. On the other hand, if $5T = 2\pi m$, we have $5 \pm 10\alpha + 10(2\alpha^2 - 1) = 0$, by letting $\alpha = \cos(\sqrt{5}T/2)$. This implies that $\alpha = (\mp 1 \pm \sqrt{5})/4$ which equals to $\cos(\pi j/5)$, for some $j \in \mathbb{Z}^+$. Since $p_0(T) = p_2(T)$, we get $\cos(\sqrt{5}T/2) = \cos(\pi j/5)$; thus, $\sqrt{5}T/2 = \pi n/5$, for some $n \in \mathbb{Z}$. Also, since $5T = 2\pi m$, we have $\sqrt{5}T/2 = \pi m/\sqrt{5}$ or $5m/n = \sqrt{5}$, which is a contradiction. □

## 5. Average Mixing

In this section, we prove that no weighted graphs are average universal mixing and show a necessary condition for a weighted graph to be average uniform mixing. But, first we prove a lemma on the average probability of the start vertex in a quantum walk on any weighted graph.

**Lemma 2** *In a quantum walk on a weighted graph $G = (V, E)$ starting at an arbitrary vertex, the average probability of the start vertex satisfies:*

$$\overline{p}_{\mathsf{start}} \geq \frac{1}{\tau(G)}. \tag{30}$$

*Proof* Since the adjacency matrix $A$ of $G$ is a real symmetric matrix, it has real eigenvalues and is real orthogonally diagonalizable (see [15]). Let $\lambda_k$ and $|v_k\rangle$ be the eigenvalues and orthonormal eigenvectors of $A$, $k = 1, \ldots, n$. Assuming that the start vertex is 0, without loss of generality, and that $|0\rangle = \sum_k \alpha_k |v_k\rangle$, for $\alpha_k \in \mathbb{R}$, we have $\sum_k \alpha_k^2 = 1$. In what follows, let $\beta_k = \alpha_k^2$. The quantum walk on $G$ is given by $|\psi(t)\rangle = \sum_k e^{-it\lambda_k}\alpha_k|v_k\rangle$. Thus, the amplitude of the start vertex at time $t$ is $\psi_0(t) = \sum_k e^{-it\lambda_k}\beta_k$; and, the average probability of the start vertex is

$$\overline{p}_0 = \lim_{T\to\infty}\frac{1}{T}\int_0^T \mathsf{d}t \sum_{j,k} e^{-it(\lambda_j - \lambda_k)}\beta_j\beta_k = \sum_{j,k} [\![\lambda_j = \lambda_k]\!]\beta_j\beta_k \tag{31}$$

$$= \sum_{\lambda \in Sp(G)}\sum_{j,k} [\![\lambda_j = \lambda_k = \lambda]\!]\beta_j\beta_k = \sum_{\lambda\in Sp(G)} B_\lambda^2, \tag{32}$$

where $B_\lambda = \sum_{j:\lambda_j=\lambda} \beta_j$. Since $\sum_\lambda B_\lambda = 1$, the last expression is minimized when $B_\lambda = 1/\tau(G)$, for each $\lambda \in Sp(G)$. Thus, the average probability of the start vertex is at least $1/\tau(G)$. □

The previous lemma has two direct implications to uniform and universal mixings. In [22], it was proved that if a circulant graph $G$ has bounded eigenvalue multiplicity then $G$ is average almost-uniform mixing. The next claim shows a partial converse to this for arbitrary weighted graphs, and thus provides a nearly tight characterization of circulant graphs that are average almost-uniform mixing. This is because if a graph has bounded eigenvalue multiplicity then it has a linear spectral type; but the converse if not known to hold, even for the case of circulant graphs.

**Corollary 2** *If a weighted graph $G = (V, E)$ is average almost-uniform mixing then $\tau(G) = O(n)$.*

*Proof* If $\tau(G) = o(n)$, then the average probability of the start vertex is $\omega(1/n)$, which implies that $G$ is not average almost-uniform mixing. □

**Corollary 3** *No weighted graphs are average universal mixing.*

*Proof* Since the average probability of the start vertex is at least $1/\tau(G)$, it is bounded away from zero. □

## 6. Conclusions

In this work, we investigate the set of probability distributions generated by a continuous-time quantum walk on weighted graphs. We show that the instantaneous probability distributions generated by a quantum walk on the weighted claw (or star) graph $K_{1,n}$ ranges over all distributions as the edge weights are varied over the non-negative real numbers. In this sense, the weighted claw has the *universal* mixing property. This is a generalization of the *uniform* mixing property on unweighted graphs considered in earlier works on the hypercube [24], the complete graphs [2], and the Cayley graph of the symmetric group [14]. Our next result shows that all complete multipartite graphs are universal mixing. This stands in contrast with the fact that unweighted complete multipartite graphs are not uniform mixing, except for the lone case of $K_{2,2}$ (see [2]). The proof of the multipartite result uses a weighted generalization of the *path collapsing* argument (from [7]). These results on instantaneous universal mixing of weighted graphs can be extended to unweighted multigraphs (where multiple edges can connect two vertices) if an approximate mixing notion is allowed.

For universal mixing over average distributions, we show that there are no graphs with this property. In fact, a key ingredient in this proof shows a necessary condition for a graph to be average almost-uniform mixing. A weighted graph is average almost-uniform mixing unless its spectral type is sublinear in the number of vertices. This provides a near tight characterization for circulant graphs, since they are known to be average almost-uniform mixing if the eigenvalues have bounded multiplicities [22]. Note that bounded eigenvalue multiplicities implies linear spectral type; but the converse is unclear, even for circulants.

A main open question left from this work is whether weighted paths $P_n$, $n \geq 4$, are instantaneous universal mixing. If the weighted paths $P_n$ are universal mixing, then so are all weighted trees; but if they are not, then an interesting question is to characterize the weighted trees that are universal mixing. A related question on weighted paths is whether they are average almost-uniform mixing, given that their spectral type is always linear (see [16]). We leave these questions for future work.

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