The tessellation problem of quantum walks

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Abstract

Quantum walks have received a great deal of attention recently because they can be used to develop new quantum algorithms and to simulate interesting quantum systems. In this work, we focus on a model called staggered quantum walk, which employs advanced ideas of graph theory and has the advantage of including the most important instances of other discrete-time models. The evolution operator of the staggered model is obtained from a tessellation cover, which is defined in terms of a set of partitions of the graph into cliques. It is important to establish the minimum number of tessellations required in a tessellation cover, and what classes of graphs admit a small number of tessellations. We describe two main results: (1) infinite classes of graphs where we relate the chromatic number of the clique graph to the minimum number of tessellations required in a tessellation cover, and (2) the problem of deciding whether a graph is $k$-tessellable for $k \geq 3$ is NP-complete.

Keywords: staggered quantum walk, clique graph, tessellation, NP-completeness

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1 Introduction

Random walks play an important role in computer science mainly in the area of algorithms and it is expected that quantum walks, which is the quantum counterpart of random walks, will play at least a similar role in quantum computation. In fact, in the last decades there has been much interest in the area of quantum walks and they are considered one of the main techniques to build algorithms for quantum computers [8].

Quantum walks on graphs come in two flavors: continuous- and discrete-time. There are more than one model for discrete-time quantum walks. The most known ones are the coined [1] and Szegedy's model [6]. Recently, a new model called staggered quantum walk [4,5] was proposed, which in some sense is more general than the previous ones because the staggered model includes the entire Szegedy’s and the most interesting instances of the coined model.

The staggered model on graphs is defined by an evolution operator that is a product of unitary matrices obtained from the graph by a tessellation process. A tessellation is a partition of the graph into cliques so that the union of the cliques covers the vertex set but not necessarily the edge set. There is a recipe to build a unitary and Hermitian matrix based on a chosen tessellation [4,5]. To define the evolution operator of the quantum walk, one has to choose extra tessellations until the tessellation union covers the edge set.

The simplest evolution operators are the product of few unitary matrices, and at least two matrices corresponding to 2-tessellable graphs are required. The class of 2-tessellable graphs was exhaustively studied in Ref. [4], which showed that a graph is 2-tessellable if and only if its clique graph is 2-colorable. Clique graphs [7] play a central role in the tessellation problem. Graphs whose clique graphs require \( k > 2 \) colors to be vertex-colored cannot be covered by just two tessellations, for example, the stars \( S_k \).

An important concept in this context is the minimum number of tessellations required to cover the graph, called the tessellation number. An upper bound is easily established by using the clique graph operator. In fact, we show that the chromatic number of the clique graph is a tight upper bound for the tessellation number. On the other hand, we obtain a class of 3-tessellable graphs whose clique graphs have arbitrarily large chromatic number, establishing the tightness of the lower bound.

Another important concept is the NP-completeness character of the tessellation problem. We show that to determine whether a graph is \( k \)-tessellable for \( k > 2 \) is NP-complete by reduction from the edge coloring problem of triangle free graphs with degree at most three [3]. The tessellation problem is also directly related to the set cover problem [2].
Preliminaries

A clique is a subset of vertices of a graph such that its induced subgraph is complete. A clique of size \( d \) is called a \( d \)-clique. In a partition of the graph into cliques, each element of the partition is a clique and two elements of the partition cannot have a vertex in common.

Definition 1.1 A tessellation \( \mathcal{T} \) is a partition of the graph into cliques, where each clique is called a polygon (or a cell), such that the union of the polygons covers the vertex set. An edge belongs to the tessellation if and only if both endpoints of the edge belong to the same polygon. The set of edges belonging to \( \mathcal{T} \) is denoted by \( E(\mathcal{T}) \).

Definition 1.2 A tessellation cover of size \( k \) of a graph \( \Gamma \) is a set of \( k \) tessellations \( \mathcal{T}_1, ..., \mathcal{T}_k \) whose union \( \bigcup_{i=1}^{k} E(\mathcal{T}_i) \) is the edge set of \( \Gamma \). The tessellation number \( T(\Gamma) \) is the cardinality of a smallest tessellation cover of \( \Gamma \). A graph \( \Gamma \) is called \( t \)-tessellable for an integer \( t \) when \( T(\Gamma) \leq t \). The \( t \)-tessellation problem asks given a graph \( \Gamma \) whether \( \Gamma \) is \( t \)-tessellable.

As an example, we illustrate the above definitions using the wheel graph, which is the graph \( W_n \) for \( n > 2 \) with vertex set \( \{0, 1, 2, ..., n\} \) and edge set \( \{\{0, n\}, \{1, n\}, ..., \{n-1, n\}, \{0, 1\}, \{1, 2\}, ..., \{n-2, n-1\}, \{n-1, 0\}\} \). Notice that \( T(W_6) = 3 \) because tessellations \( \mathcal{T}_0 = \{\{0\}, \{3\}, \{1, 2\}, \{4, 5, 6\}\} \), \( \mathcal{T}_1 = \{\{1\}, \{4\}, \{0, 5\}, \{2, 3, 6\}\} \), \( \mathcal{T}_2 = \{\{2\}, \{5\}, \{3, 4\}, \{0, 1, 6\}\} \) form a minimum tessellation cover. In fact, each of \( \mathcal{T}_0, \mathcal{T}_1, \) and \( \mathcal{T}_2 \) is a partition into cliques which covers all vertices. The set \( E(\mathcal{T}_0) \cup E(\mathcal{T}_1) \cup E(\mathcal{T}_2) \) is equal to the edge set of \( W_6 \), and it is not possible to cover the edge set with less than three tessellations because a tessellation of \( W_6 \) can cover at most two edges incident to vertex 6.

Definition 1.3 A coloring (resp. an edge-coloring) of a graph is a labeling of vertices (edges) with colors such that no two adjacent vertices (incident edges) have the same color. A \( k \)-colorable (\( k \)-edge-colorable) graph is the one whose vertices (edges) can be colored with at most \( k \) colors so that no two adjacent vertices (edges) share the same color. The chromatic number \( \chi(\Gamma) \) (chromatic index \( \chi'(\Gamma) \)) of a graph \( \Gamma \) is the smallest number of colors needed to color the vertices (edges) of \( \Gamma \).

2 Results

How far from \( \chi(K(\Gamma)) \) is \( T(\Gamma) \)?

In this subsection, we relate the tessellation number to some non-trivial classes of graphs and we prove the following proposition.
Proposition 2.1 Let $\Gamma$ be a graph whose clique graph is not 2-colorable. Then, $3 \leq T(\Gamma) \leq \chi(K(\Gamma))$.

Proof The lower bound $3 \leq T(\Gamma)$ is a direct consequence of the fact that a graph is 2-tessellable if and only if its clique graph is 2-colorable, proved in Ref. [4]. Now we give a proof for the upper bound $T(\Gamma) \leq \chi(K(\Gamma))$. We define a family of $\chi(K(\Gamma))$ tessellations whose union covers the edges of graph $\Gamma$ as follows. Consider an optimal coloring of $K(\Gamma)$, and let $S_g$ be the set of maximal cliques corresponding to the vertices of $K(\Gamma)$ colored by color $g$. Any pair of such maximal cliques must be disjoint, so we can define a tessellation $T_g$ whose polygons are the cliques of $S_g$ together with missing vertices of $\Gamma$. Since every edge of $\Gamma$ belongs to at least one maximal clique, the union of the $\chi(K(\Gamma))$ defined tessellations covers the edges of graph $\Gamma$, as required in order to establish the upper bound.

Now we show that both bounds of Proposition 2.1 are tight. Next Proposition shows that the upper bound is tight.

Proposition 2.2 Let $\Gamma$ be the windmill graph with $\ell$ maximal cliques $C_1, C_2, \ldots, C_\ell$ such that the intersection of $C_1, C_2, \ldots, C_\ell$ is precisely one vertex $u$. Then, $T(\Gamma) = \chi(K(\Gamma)) = \ell$.

Proof The clique graph of $\Gamma$ is the complete graph with $\ell$ vertices. Hence, by Proposition 2.1, $\ell$ is an upper bound for $T(\Gamma)$. On the other hand, it is not possible to cover the edge set with less than $\ell$ tessellations, since each tessellation cannot cover the edges of more than one maximal clique $C_i$.

The tightness of the lower bound is revealed by the following class of graphs.

Definition 2.3 The (3, $n$)-extended wheel graph $E_{3,n}$ for $n \geq 2$ is defined by adding to the wheel graph $W_{3n}$ the following edges: $\{3i, 3j\}, \{3i+1, 3j+1\}$ and $\{3i+2, 3j+2\}$, for $0 \leq i < j < n$.

Proposition 2.4 The maximal cliques of $E_{3,n}$ are 3-cliques or $(n+1)$-cliques. The number of maximal cliques is $3n+3$. The maximal cliques are the 3-cliques of the spanning wheel $W_{3n}$, plus three new $(n+1)$-cliques. All maximal cliques share the vertex with label $3n$.

Proof Let $i$ be an index in the range $0 \leq i < 3n$ and the arithmetic with this index be performed modulo $3n$. Then, the set $\{i, i+1, 3n\}$ is a maximal 3-clique because it induces a triangle of the spanning wheel graph and in $E_{3,n}$ the set of vertices $\{i, 0 \leq i < 3n\}$ contains no 3-clique. Now consider the three sets of vertices $\{0, 3, 6, \ldots, 3n - 3, 3n\}$, $\{1, 4, 7, \ldots, 3n - 2, 3n\}$, and
{2, 5, 8, ..., 3n − 1, 3n}, each of them with cardinality (n + 1). We claim that each one is a maximal (n + 1)-clique. Consider the set \{0, 3, 6, ..., 3n − 3, 3n\} (analogous for the other ones). All vertices in this set are adjacent because the edges are either \{3i, 3j\} for some 0 ≤ i, j < n or \{3i, 3n\} for some 0 ≤ i < n. In the first case, these edges were added to \(W_{3n}\) to define \(E_{3.n}\), and in the second case the edges belong to the spanning wheel graph. If a new vertex is added, the new vertex must have the form \(3i + 1\) or \(3i + 2\) for some \(0 ≤ i < n\) and it will not be adjacent to all vertices of set \{0, 3, 6, ..., 3n − 3, 3n\}. Then, this set is a maximal clique. There are three such \((n + 1)\)-maximal cliques and there are no other maximal cliques. Then, the total number of maximal cliques is \(3n + 3\) and all of them share the vertex with label \(3n\).

It follows from Proposition 2.4 that \(K(E_{3,n})\) is the complete graph with \(3n+3\) vertices, and hence Proposition 2.1 establishes the upper bound \(T(E_{3,n}) ≤ 3n + 3\). We prove next that the actual value of \(T(E_{3,n})\) is much smaller.

**Proposition 2.5** \(T(E_{3,n}) = 3\) for \(n ≥ 2\).

**Proof** Let us show that \(E_{3.n}\) is 3-tessellable by describing explicitly three tessellations that cover the edges of \(E_{3,n}\). The tessellations are the following ones:

\[
\begin{align*}
\mathcal{T}_0 &= \{0, 3, 6, ..., 3n - 3, 3n\}, \{3i + 1, 3i + 2\} \text{ for } 0 ≤ i ≤ n - 1, \\
\mathcal{T}_1 &= \{1, 4, 7, ..., 3n - 2, 3n\}, \{3i + 2, 3i + 3\} \text{ for } 0 ≤ i ≤ n - 1, \\
\mathcal{T}_2 &= \{2, 5, 8, ..., 3n - 1, 3n\}, \{3i + 3, 3i + 4\} \text{ for } 0 ≤ i ≤ n - 1,
\end{align*}
\]

where the arithmetic with index \(i\) is performed modulo \(3n\). Let us show that \(\mathcal{T}_0\) is a well defined tessellation (analogous for the other ones) by checking each item of the following list: (1) Each polygon in \(\mathcal{T}_0\) must be a clique, (2) the polygons in \(\mathcal{T}_0\) must be pairwise disjoint, and (3) the union of the polygons in \(\mathcal{T}_0\) must be the vertex set. By using the proof of Proposition 2.4 and the fact that \(\{3i + 1, 3i + 2\}\) is an edge of the spanning wheel, we check item (1). Using that set \(\{0, 3, 6, ..., 3n - 3, 3n\}\) is comprised of vertices that are multiple of 3 while no vertex in sets \(\{3i + 1, 3i + 2\}\) for \(0 ≤ i ≤ n - 1\) is multiple of 3, we check item (2). The union of the sets in \(\mathcal{T}_0\) is the vertex set, and we check item (3). Since no edge belongs to more than one tessellation and each tessellation covers \(n(n + 3)/2\) edges, the union \(\mathcal{E}(\mathcal{T}_0) \cup \mathcal{E}(\mathcal{T}_1) \cup \mathcal{E}(\mathcal{T}_2)\) covers \(3n(n + 3)/2\) edges, which is the number of edges of \(E_{3,n}\). It is not possible to cover the edges of \(E_{3,n}\) with less than three tessellations because the chromatic number of the clique graph of \(E_{3,n}\) is larger than 2. Then, \(T(E_{3,n}) = 3\) for \(n ≥ 2\). \(\square\)
3-tessellation is NP-complete
Deciding whether a graph is \( k \)-tessellable for \( k \geq 3 \) is NP-complete. To prove this statement, we use the class of triangle-free graphs with maximum vertex degree 3 because the 3-edge-coloring problem in this class is NP-complete [3].

**Theorem 2.6** Deciding whether a graph is 3-tessellable is NP-complete.

**Proof** In a triangle-free graph \( \Gamma \), a 3-tessellation corresponds to 3 matchings of \( \Gamma \) covering its edge set, and so define a 3-edge-coloring of \( \Gamma \).

\[ \square \]

**Final remarks**
We have shown that the lower bound of \( T(\Gamma) \) does not depend on \( \chi(K(\Gamma)) \), at least when \( \chi(K(\Gamma)) \) is multiple of 3. Besides classes \( E_{3,n} \) and the windmill graphs for which we were able to establish tessellation numbers satisfying \( T(\Gamma) = 3 \) and \( T(\Gamma) = \chi(K(\Gamma)) \), respectively, we were able to define additional infinite classes of graphs satisfying \( \frac{T(\Gamma)}{\chi(K(\Gamma))} \in \{\frac{1}{2}, \frac{1}{3}, \frac{1}{4}\} \), \( T(\Gamma) = \sqrt{\chi(K(\Gamma))} \), and further ones obtained by extending \( E_{3,n} \) into \( E_{k,n} \) for \( k \geq 4 \).

For every graph \( \Gamma \), is there a minimum tessellation cover such that every tessellation contains a polygon which is a maximal clique of \( \Gamma \)?

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Appendix: Example of some class of graphs $\Gamma$ and their tessellation number $T(\Gamma)$

We should mention that in order to obtain some of the infinite classes of graphs presented below, we have used the following computational approach. Let $\mathcal{S}$ be the set of all tessellations $\{T_1, ..., T_r\}$ of a graph $\Gamma$. Define the set $\mathcal{E}(\mathcal{S}) = \{\mathcal{E}(T_1), ..., \mathcal{E}(T_r)\}$. A minimum tessellation cover of $\Gamma$ corresponds to a minimum set cover [2] for $\mathcal{E}(\mathcal{S})$. This approach for finding the minimum tessellation cover is highly inefficient mainly because the cardinality of $\mathcal{S}$ is too large. It is possible to reduce the size of $\mathcal{S}$ by selecting tessellations that contain at least one maximal clique. This algorithm is not exhaustive but is efficient enough when we use greedy algorithms for the set cover problem.

Class with $T(\Gamma) = \chi(K(\Gamma))$.

Figure 1. The class of windmill graphs considered in Proposition 2.2 is a tight graph class with respect to the upper bound of Proposition 2.1. The windmill $\Gamma$ has 5 triangles, its clique graph $K(\Gamma)$ is the complete graph with 5 vertices, and the tessellation number $T(\Gamma)$ is 5.
Class with $\frac{T(\Gamma)}{\chi(K(\Gamma))} = \frac{1}{2}$.

Figure 2. The class of wheel graphs. In the example, the wheel $\Gamma = W_6$ has 7 vertices, its clique graph $K(\Gamma)$ is the complete graph with 6 vertices, and the tessellation number $T(\Gamma)$ is 3. A 3-tessellation cover is highlighted by using 3 colors.

Class with $\frac{T(\Gamma)}{\chi(K(\Gamma))} = \frac{1}{3}$.

Figure 3. In the example, the graph $\Gamma$ contains the wheel $W_6$ as a spanning subgraph, its clique graph $K(\Gamma)$ is the complete graph with 9 vertices, and the tessellation number $T(\Gamma)$ is 3. A 3-tessellation cover is highlighted by using 3 colors.
Class with \( \frac{T(\Gamma)}{\chi(K(\Gamma))} = \frac{1}{4} \).

Figure 4. In the examples, the graphs \( \Gamma \) contain respectively the wheels \( W_{12} \) and \( W_{16} \) as a spanning subgraph. The clique graphs \( K(\Gamma) \) are respectively the complete graphs \( K_{24} \) and \( K_{32} \), and the tessellation numbers \( T(\Gamma) \) are respectively 6 and 8. The corresponding minimum tessellations are highlighted.

Class with \( T(\Gamma) = \sqrt{\chi(K(\Gamma))} \).

Figure 5. In the example, the graph \( \Gamma \) contains the wheel \( W_{10} \) as a spanning subgraph, its clique graph \( K(\Gamma) \) is the complete graph with 25 vertices, and the tessellation number \( T(\Gamma) \) is 5. A 5-tessellation cover is highlighted by using 5 colors.
Graph with $T(\Gamma) < \sqrt{\chi(K(\Gamma))}$.

Figure 6. Tessellations of a graph $\Gamma$ with $T(\Gamma) = 4$ and $\chi(K(\Gamma)) = 30$.

Class $E_{3,n}$ with $T(\Gamma) = 3$ and $\chi(K(\Gamma)) = 3n + 3$.

Figure 7. The class of extended wheel graphs considered in Proposition 2.5. The extended wheel graph $\Gamma = E_{3,4}$ has three 5-cliques and twelve 3-cliques, hence its clique graph $K(\Gamma)$ is the complete graph with 15 vertices.