ALGEBRAIC COMBINATORICS

Krystal Guo & Vincent Schmeits

Perfect state transfer in quantum walks on orientable maps
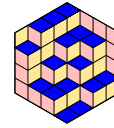
Perfect state transfer in quantum walks on orientable maps

Krystal Guo & Vincent Schmeits

ABSTRACT A discrete-time quantum walk is the quantum analogue of a Markov chain on a graph. We show that the evolution of a general discrete-time quantum walk that consists of two reflections satisfies a Chebyshev recurrence, under a projection. We apply this to study perfect state transfer in a model of discrete-time quantum walk whose transition matrix is given by two reflections, defined by the face and vertex incidence relations of a graph embedded in an orientable surface, proposed by Zhan [*J. Algebraic Combin.* 53(4):1187–1213, 2020]. For this model, called the vertex-face walk, we prove results about perfect state transfer and periodicity and give infinite families of examples where these occur. In doing so, we bring together tools from algebraic and topological graph theory to analyze the evolution of this walk.

1. Introduction

Quantum computing gives rise to many interesting applications of combinatorics; in this paper, we bring together ideas from algebraic and topological graph theory to study properties, including state transfer and periodicity, of a model of quantum walk which takes place on an embedded graph. Like their continuous-time counterpart, discrete-time quantum walks are computational primitives; [21] shows that the discrete-time quantum walk is able to implement the same universal gate set and thus any quantum algorithm can be viewed as a discrete-time quantum walk. See [25] for connections between quantum walks and quantum search. In recent papers and a recent book, Godsil and Zhan [16, 31, 17] describe the various models of discrete-time quantum walks and apply techniques from algebraic graph theory to study properties of the evolution of these walks. In this paper, we prove a result about a general model of discrete walks, where the transition matrix consists of two reflections, as well as results about perfect state transfer and periodicity in one specific model, the vertex-face model.

The quantum walks studied here are discrete-time and they are built from two reflections; the transition matrix U is of the form

$$U = (2P - I)(2Q - I),$$

where P, Q are the orthogonal projectors onto two subspaces, as defined in [22]. These walks are referred to as *bipartite walks* in [5] and are a general model of quantum walk which encompasses the walks defined by Szegedy in his seminal paper [28] and also includes the *vertex-face walks* which are the focus of this paper. In the field of quantum algorithms, study of this model is motivated by the folkloric fact that implementing
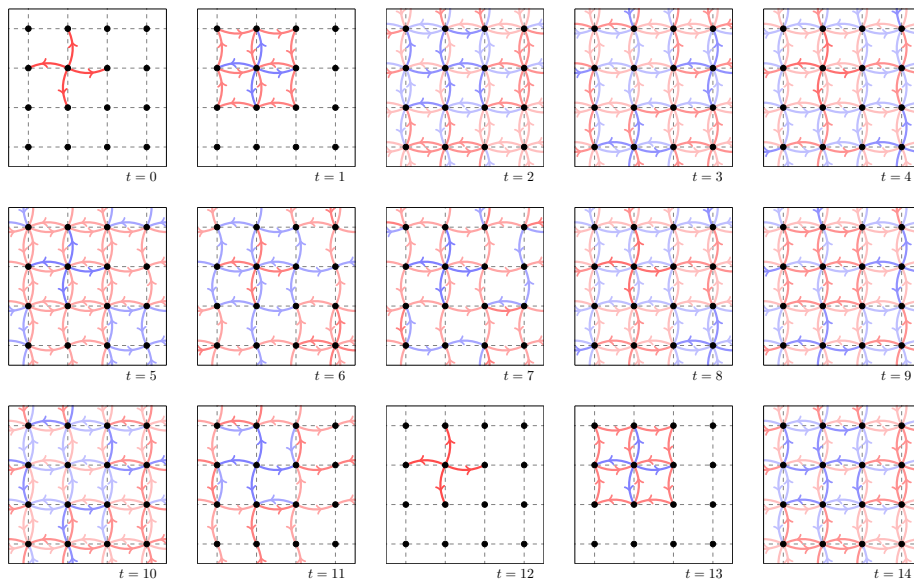
FIGURE 1. The vertex-face walk on the toroidal $(4, 4)$-grid. Each diagram consists of the 4×4 grid (which is isomorphic to $C_4 \square C_4$) embedded in the torus, shown here as a cut-open torus, where the opposite sides are identified; for visual simplicity, we have omitted the labels on the boundary of the torus. The state space of the walk is indexed by the set of arcs. Here we represent the amplitude of each arc by using opacity for magnitude and colours (red, blue) for the sign (positive, negative, resp.). The walk admits periodicity at time 12.

this model is only as hard as implementing measurements in the vector spaces onto which P and Q project; an example of a precise formulation of this occurs in [20, Claim 3.16]. For background on the role of discrete-time quantum walks in quantum algorithms, we refer to [27, 2]. We will defer the definition of the vertex-face walk until Section 3; intuitively, the walk evolves on a graph embedded in an orientable surface (also known as a *map*) and the transition matrix has the property that P and Q are the projections onto vector spaces determined by incidence relations of arcs with faces and vertices, respectively. In [24, 12, 1], the quantum walk corresponding to their spatial quantum search corresponds, in some way, to the vertex-face walk on the toroidal grids. This provided the motivation for the definition of the vertex-face model in [31]. In this work, we build upon these ideas; we provide rigorous definitions of the incidence matrices, using more context in topological graph theory, and eventually revisit the toroidal grids.

Figure 1 shows the evolution of the vertex-face walk on the toroidal $(4, 4)$-grid; the visualisation of these walks, as processes on embedded graphs, is one of the advantages of the vertex-face walk. One of the reflections of this model, defined by the arc-vertex incidence matrix, is common to multiple models of discrete quantum walks, including that of Szegedy in [28]. The second reflection is the analogous object, in the dual of the embedded graph. This allows us to use tools from topological graph theory. In particular, the census of highly symmetric maps of Conder [9] provides a plethora of examples, which is important for a new concept in a nascent field.

We describe computations that we have performed on the census in Section 8. The main observation from these computations is that, occasionally, some power of the transition matrix U is equal to the identity matrix; we only observed this behaviour for U^t where $t = 1, 2, 6, 12$. Sections 5 and 7 are devoted to explicating this behaviour. We lay the foundation for the establishment of relations between topological properties and properties of the quantum walk, which we discuss further in Section 9.

We will now give an intuitive description of the quantum walk properties studied herein, and defer rigorous definitions until Section 4. In Figure 1, we see that the states at times $t = 0$ and $t = 12$ are identical; this behaviour is called *periodicity*. If the state had moved to the same distribution, but at another vertex, it would be an example of *perfect state transfer*. Though state transfer and periodicity have been studied in continuous-time quantum walks in a combinatorial setting, see [15, 10, 14] for examples, it is a relatively unexplored topic for bipartite walks and for the vertex-face walk in particular, though some recent papers have appeared; for example, pretty good state transfer in discrete quantum walks has been studied in [4]. The relationship between continuous and discrete quantum walks is explicated in [6]. We make our own contribution by establishing some fundamental properties of state transfer in the vertex-face model of discrete-time quantum walks, with some analogous theorems to those for continuous-time quantum walks.

We now give a summary of the main results in this paper. First, we consider the general model of discrete-time quantum walks and we give a surprising Chebyshev recurrence for its evolution with respect to one of the reflections, in Theorem 4.1. By applying this recurrence to the vertex-face walk, we establish fundamental properties of perfect state transfer in Theorem 4.5. We show that, loosely speaking, if the walk admits perfect state transfer everywhere, then it also admits periodicity and has the property that there is some $\tau > 0$ such that $U^\tau = I$. We give new examples of perfect state transfer in infinite families of embeddings (dipoles and grids). Finally, we fully characterise embeddings for which $U^\tau = I$ for $\tau = 1, 2$, and give partial results for larger τ. We have performed computations on all orientably-regular maps with at most 1000 edges, and it seems that, for these maps, periodicity can only occur with period $1, 2, 6$ or 12, which is partially supported by our results.

We now discuss the organisation of this paper. Since the vertex-face walk takes place on a cellularly embedded graph, and is defined with incidence matrices which are not standard in the literature, we give the necessary preliminaries on maps in Section 2. In Section 3, we give the formal definition of the vertex-face quantum walk. In Section 4, we prove a general result about a Chebyshev recurrence for discrete-time quantum walks, and apply it in the specific model, the vertex-face walk, to prove our main results on perfect state transfer. We move to more symmetric maps in Section 5 and establish the connection between perfect state transfer, periodicity and maps for which some power of the transition matrix equals the identity matrix. We then give three infinite families of examples of perfect state transfer in Section 6. In Section 7, we work towards proving a conjecture on periodicity in orientably-regular maps. Since the vertex-face walk is a relatively new concept and not many examples are well-understood, we performed computations pertaining to our main results on the census of regular maps, as given by Conder in [8], in Section 8, to gain intuition on the behaviour these walks. Finally, we conclude with open problems in Section 9.

2. Preliminaries

Before we can give the formal definition of a vertex-face walk, we have to refresh our definitions and notation for graph embeddings. The vertex-face walk is defined for a graph embedded in an orientable surface, using the incidence relations between
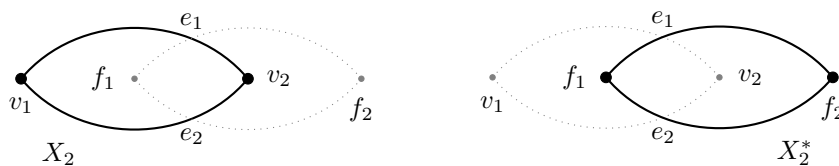
FIGURE 2. X_2 and its dual X_2^* embedded in the sphere.

its vertices, faces and edges. We allow graphs to have loops and parallel edges; we will use 'graph' and 'multigraph' interchangeably. At the end of the section, we turn our attention to automorphisms of maps and define (orientably-)regular maps, which provide a broad class of examples that can be searched computationally in order to gain intuition on vertex-face walks.

We consider cellular embeddings of graphs on orientable surfaces. A *map* is a 2-cell embedding of a connected graph into a compact, connected surface. Loosely speaking, the faces of a 2-cell embedding are homeomorphic to disks and the embedding determines the surface, which allows us to conflate properties of the underlying surface with the map itself. For background on maps, surfaces and topological graph theory, we refer the reader to [18] and [23].

A map is completely determined by its facial boundary walks. A map is *orientable* if the underlying surface is orientable. In this paper, we will exclusively consider orientable maps and will often write 'map' instead of 'orientable map' for convenience. The number of handles is called the *genus* of the surface. The *genus g* of an orientable map is equal to the genus of its underlying surface and satisfies *Euler's formula*:

$$|V| - |E| + |F| = 2 - 2g,$$

where V, E and F are respectively the sets of vertices, edges and faces of the map.

In an orientable surface, we can make a consistent distinction between a 'clockwise' and an 'anticlockwise' orientation. For each vertex of an orientable map, we can give a cyclic ordering of the edges and faces incident to that vertex, using the clockwise order in which these edges and faces are attached to that vertex. For example, for v_1 of the embedded digon in Figure 2, the order is (e_1, f_1, e_2, f_2). The subsequence of edges is said to be the *rotation* of the vertex and the set of all rotations forms the *rotation system* of the map. Every orientable map is, up to homeomorphism, uniquely defined by its rotation system. Note that every edge e appears twice in the rotation system; if e is a loop, it will appear twice in the rotation of a single vertex. With the clockwise orientation, the edges incident to a face can be ordered similarly; the *facial walk* is the alternating sequence of incident vertices and edges in the clockwise order in which they appear on the boundary of that face. For the example shown in Figure 2, the facial walk of f_1 of X_2 is given by (v_1, e_1, v_2, e_2). Note that a face (resp. vertex) can appear more than once on the same rotation (resp. facial walk) (Figure 5 illustrates this).

The *dual X^** of a map X is the map whose vertex set is the set of faces of X, whose edge set is equal to that of X, and whose rotation system is given by the set of facial walks of X. Note that the dual is also a 2-cell embedding in the same surface. Figure 2 depicts the digon (left) and its dual (right) embedded in the sphere (genus 0). We will denote the digon by X_2. We have $V = \{v_1, v_2\}$, $E = \{e_1, e_2\}$ and $F = \{f_1, f_2\}$. Note that X_2 is *self-dual*: there exist bijections $V \to F$ and $E \to E$ that preserve the incidence structure of the map. (In particular, the graphs underlying the map and its dual are isomorphic.)
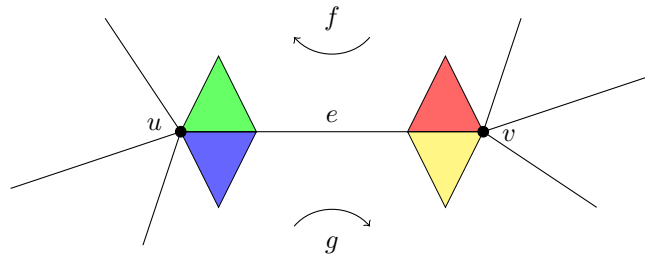
FIGURE 3. The coloured triangles represent the flags that are incident to the edge e. The blue and red flags are the clockwise flags. The arced arrows indicate the clockwise orientations of the facial walks.

The *(vertex-)degree* of a vertex is the number of edges in its rotation. Note that each loop contributes 2 to the degree of the vertex that it is attached to. Likewise, the *(face-)degree* of a face is the number of edges in its facial walk. If an edge appears twice in the facial walk (which implies that it is a loop in the dual), then it contributes 2 to the face-degree. A *type* (k, d) map is a map where every vertex has degree d and every face has degree k. The dual of a type (k, d) map is a type (d, k) map. The map X_2 is a type $(2, 2)$ map.

Let X be a map and assume, at first, that both X and its dual have no loops. A *flag* of X is defined as a triple (v, e, f) of a vertex v, an edge e and a face f of X that are all pairwise incident to each other. The set of all flags is denoted by $\mathcal{F}$ and we have $|\mathcal{F}| = 4|E|$, as every edge is incident to four distinct flags. For example, in Figure 3, the green triangle represents the flag (u, e, f). In the example in Figure 2, the flags are formed by all possible triples:

$$(v_1, e_1, f_1), (v_1, e_2, f_1), (v_1, e_2, f_2), (v_1, e_1, f_2),$$
$$(v_2, e_2, f_1), (v_2, e_1, f_1), (v_2, e_1, f_2), (v_2, e_2, f_2).$$

Since X is orientable, we can make a distinction between flags that are clockwise and flags that are anticlockwise, by the direction in which the flag 'points'. More precisely, we say that a flag (v, e, f) is *clockwise* (resp. *anticlockwise*) if, in the clockwise (resp. anticlockwise) orientation of the facial walk of f, the edge e follows v. In Figure 3, the blue and red flags are the clockwise flags, and the green and yellow flags are oriented anticlockwise. The clockwise flags in Figure 2 are

$$(v_1, e_1, f_1), (v_1, e_2, f_2), (v_2, e_2, f_1), (v_2, e_1, f_2).$$

Given an orientable map X, we can, for every non-loop edge, add a pair of arcs pointing in opposite directions, and positioned on opposite sides of that edge. As such, each arc lies inside a face of X. Because of the orientability of X, this can be done in such a way that each arc is pointed in the direction of the facial walk of its corresponding face. We denote the set of arcs by $\mathcal{A}$. In Figure 4, the arcs of X_2 are depicted.

For our initial definition of a flag, we assumed that both X and its dual have no loops. In that case, there is a clear 1-1 correspondence between the arcs of X and its clockwise flags. For example, in Figure 4, the arc a_1 corresponds to the flag (v_2, e_1, f_2): the tail of a_1 is v_2, and the arc lies inside f_2, alongside the edge e_1. If X or its dual X^* has a loop, however, we require a more abstract definition which allows for multiple flags to be incident to the same triple (v, e, f). We define the set of flags $\mathcal{F}$ to be an abstract set with an incidence function $\phi : \mathcal{F} \to V \times E \times F$, such that every edge e is incident to four unique flags. Intuitively, we would like the four flags shown in
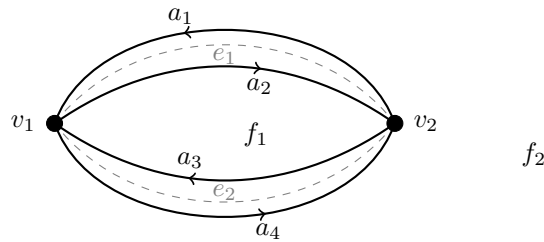
FIGURE 4. The arcs of X_2. Note that the spaces between arcs a_1 and a_2 and between arcs a_3 and a_4 do not depict new faces; rather, each arc lies inside f_1 or f_2.
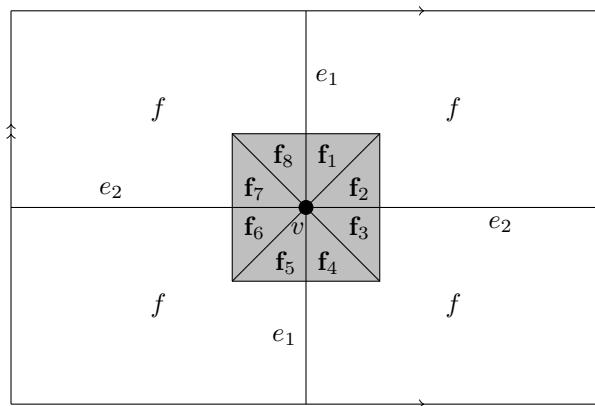

FIGURE 5. One vertex with two loops embedded in the torus, shown as a cut-open torus. It has 8 flags. The rotation around v is given by $(e_1, f, e_2, f, e_1, f, e_2, f)$ and the facial walk of f is $(e_1, v, e_2, v, e_1, v, e_2, v)$.

Figure 3 to be distinct objects. Figure 5 shows a graph consisting of a single vertex with two loops attached, embedded as an orientable map on the torus. It has a single vertex v and a single face f, so $|V \times E \times F| = 2$. The flags $\mathbf{f}_1$, $\mathbf{f}_4$, $\mathbf{f}_5$ and $\mathbf{f}_8$ are incident to the triple (v, e_1, f) and the flags $\mathbf{f}_2$, $\mathbf{f}_3$, $\mathbf{f}_6$ and $\mathbf{f}_7$ are incident to (v, e_2, f). The clockwise flags are $\mathbf{f}_1$, $\mathbf{f}_3$, $\mathbf{f}_5$ and $\mathbf{f}_7$, and they correspond to the arcs of the map.

Given an orientable map X, we need to define several incidence matrices; the state space for the quantum walk that we study is indexed by the set of arcs of the map. For an arc $a \in \mathcal{A}$, let $v(a)$ be the tail vertex of a, let $f(a)$ be the face in which a lies, and let $e(a)$ be the edge along which a lies. (Alternatively, $(v(a), e(a), f(a))$ is the incident triple for the corresponding clockwise flag.) We define the *arc-vertex incidence matrix* $N \in \{0, 1\}^{\mathcal{A} \times V}$, the *arc-face incidence matrix* $M \in \{0, 1\}^{\mathcal{A} \times F}$ and the *arc-edge incidence matrix* $L \in \{0, 1\}^{\mathcal{A} \times E}$ as follows:

$$N(a, v) = \begin{cases} 1 & \text{if } v = v(a); \\ 0 & \text{otherwise,} \end{cases} \quad M(a, f) = \begin{cases} 1 & \text{if } f = f(a); \\ 0 & \text{otherwise,} \end{cases} \quad \text{and}$$

$$L(a, e) = \begin{cases} 1 & \text{if } e = e(a); \\ 0 & \text{otherwise.} \end{cases}$$

The incidence matrices for X^* (with the same set of arcs $\mathcal{A}$) are obtained by reversing the roles of N and M. Note that these are different incidence matrices from those often considered in the literature; these incidence matrices capture incidence relations on arcs, instead of incidence relations on edges. For the map X_2, the matrices can be written down explicitly as follows:

$$
N = \begin{array}{c} \\ a_1 \\ a_2 \\ a_3 \\ a_4 \end{array} \overset{\displaystyle v_1 v_2}{\begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{bmatrix}}, \qquad
M = \begin{array}{c} \\ a_1 \\ a_2 \\ a_3 \\ a_4 \end{array} \overset{\displaystyle f_1 f_2}{\begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}}, \quad \text{and} \quad
L = \begin{array}{c} \\ a_1 \\ a_2 \\ a_3 \\ a_4 \end{array} \overset{\displaystyle e_1 e_2}{\begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}}.
$$

For any arc $a \in A$, we denote by $\overleftarrow{a}$ the unique other arc incident to the edge $e(a)$; that is, $\overleftarrow{a}$ is the arc going in the opposite direction from a. For instance, in Figure 4, $\overleftarrow{a_1} = a_2$. The *arc-reversal matrix* $R \in \{0,1\}^{\mathcal{A} \times \mathcal{A}}$ is the permutation matrix that swaps each such pair of arcs: it is defined by

$$
R(a,b) = \begin{cases} 1 & \text{if } \overleftarrow{a} = b; \\ 0 & \text{otherwise.} \end{cases}
$$

Alternatively, we can write $R = LL^T - I$. In the case of our example X_2, the matrix R is given by

$$
R = I_2 \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.
$$

Let $D \in \mathbb{C}^{V \times V}$ be the diagonal matrix for which the diagonal (v, v)-entry is equal to the degree of the vertex v. Similarly, let $\Delta \in \mathbb{C}^{F \times F}$ be the diagonal matrix for which the diagonal (f, f)-entry is equal to the degree of the face f. The following properties hold:

$$(1) \qquad\qquad N^T N = D, \quad L^T L = 2I \quad \text{and} \quad M^T M = \Delta;$$

$$(2) \qquad\qquad N^T R N = A(X) \quad \text{and} \quad M^T R M = A(X^*);$$

Here, $A(X)$ denotes the adjacency matrix of the graph underlying the map X. The properties in (1) are trivial. Equations similar to the equation on the left in (2) are easily derived and have appeared in other texts (although they often involve edge-vertex incidences, rather than arc-vertex incidences), see for instance [13]. The equation on the right then follows from duality.

The matrix $C := N^T M$ is the *vertex-face incidence matrix* of X; the (v, f)-entry of C is equal to the number of times that the vertex v appears on the facial walk of f. If we had defined the facial walks to be oriented in the anticlockwise direction, then RM would have been the arc-face incidence matrix of the map, but the entries of C do not depend on the orientation, hence

$$(3) \qquad\qquad N^T R M = N^T M.$$

An orientable map X has *incidence multiplicity* α if, whenever a vertex appears on the facial walk of a face, it appears on that face exactly α times. Equivalently, X has incidence multiplicity α if all non-zero entries of C are equal to α. If $\alpha = 1$ and all facial walks have length at least 3, then we say that X is *circular*; in this case, every facial walk is a cycle in the graph underlying X. For the example X_2 of the embedded digon, we have

$$
C = \begin{array}{c} \\ v_1 \\ v_2 \end{array} \overset{\displaystyle f_1 f_2}{\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}},
$$

and thus X_2 is an example of a map with incidence multiplicity 1, but it is not circular.

By construction, each of the matrices N and M has pairwise orthogonal columns. For the vertex-face quantum walk we need to consider the normalized versions of these incidence matrices; we define

$$\widehat{N} := ND^{-\frac{1}{2}} \quad \text{and} \quad \widehat{M} := M\Delta^{-\frac{1}{2}}$$

to be the *normalized arc-vertex* and *arc-face incidence matrices*, respectively. The sets of columns of $\widehat{N}$ and $\widehat{M}$ form orthonormal bases for the column spaces of N and M respectively. From (1) and (3), we obtain the following identities:

$$\widehat{N}^T \widehat{N} = \widehat{M}^T \widehat{M} = I; \tag{4}$$

$$\widehat{N}^T R \widehat{M} = \widehat{N}^T \widehat{M}. \tag{5}$$

We also define

$$\widehat{C} := \widehat{N}^T \widehat{M} = D^{-\frac{1}{2}} C \Delta^{-\frac{1}{2}}$$

to be the *normalized vertex-face incidence matrix*.

An *automorphism* of a map X, orientable or non-orientable, is a permutation of the flags of X that preserves all incidences between flags, vertices, edges and faces. We denote the group of automorphisms of X by $\mathrm{Aut}(X)$. Every automorphism is completely determined by the image of any single flag. Thus if the action of $\mathrm{Aut}(X)$ on $\mathcal{F}$ is transitive, it is regular. In that case, we say that X is a *(fully) regular map*. Specifically, if such a map X is orientable, it is called *reflexible*. If X is orientable and the action of $\mathrm{Aut}(X)$ on the flags has two orbits (instead of one), which are the sets of clockwise and anticlockwise flags, then X is a *chiral map*. An *orientably-regular map* is an orientable map that is either reflexible or chiral. Though some definitions vary among the literature, our nomenclature is consistent with the census of regular maps [8, 9], which we used for or computations in Section 8.

Each automorphism of X induces permutations of the vertices, edges and faces, preserving incidences. We record these in the following proposition, for use in later sections.

PROPOSITION 2.1. *Suppose that π is an automorphism of X and write $\pi_{\mathcal{A}}$, π_V, π_E and π_F for the permutation matrices that correspond to the action of π on the sets of clockwise flags, vertices, edges and faces of X respectively. Then*

(i) $\pi_{\mathcal{A}} N = N \pi_V$;
(ii) $\pi_{\mathcal{A}} L = L \pi_E$; *and*
(iii) $\pi_{\mathcal{A}} M = M \pi_F$. □

Clearly, the actions of $\mathrm{Aut}(X)$ on the sets V, E and F are transitive if X is orientably-regular.

With these preliminaries in mind, we will retain the definitions of M, N, R and $\mathcal{A}$ for a map X for the rest of the paper, unless specifically stated otherwise.

3. Vertex-face quantum walk

In this section, we define the vertex-face quantum walk and state the existing results.

Suppose that X is an orientable map, and that N is its arc-vertex incidence matrix and M its arc-face incidence matrix. Let $Q, P \in \mathbb{C}^{\mathcal{A} \times \mathcal{A}}$ be the orthogonal projections onto the column spaces of N and M respectively. Note that we can write

$$Q = \widehat{N} \widehat{N}^T \quad \text{and} \quad P = \widehat{M} \widehat{M}^T,$$

where $\widehat{N}$ and $\widehat{M}$ are the respective normalized incidence matrices, because the columns of $\widehat{N}$ and $\widehat{M}$ form respective orthonormal bases for $\mathrm{col}(N)$ and $\mathrm{col}(M)$. We speak of

the column spaces of N and $\widehat{N}$ interchangeably, and do the same for M and $\widehat{M}$. For readability we will often, if possible, use just N and M instead of their normalized versions. For instance, if X is a type (k, d) map, we can write

$$Q = \frac{1}{d} N N^T \quad \text{and} \quad P = \frac{1}{k} M M^T.$$

For our example of the embedded digon X_2, as defined in the previous section, the matrices Q and P are given as follows:

$$Q = \frac{1}{2} \begin{bmatrix} 1\ 0\ 1\ 0 \\ 0\ 1\ 0\ 1 \\ 1\ 0\ 1\ 0 \\ 0\ 1\ 0\ 1 \end{bmatrix} \quad \text{and} \quad P = \frac{1}{2} \begin{bmatrix} 1\ 0\ 0\ 1 \\ 0\ 1\ 1\ 0 \\ 0\ 1\ 1\ 0 \\ 1\ 0\ 0\ 1 \end{bmatrix}.$$

Let $U \in \mathbb{C}^{\mathcal{A} \times \mathcal{A}}$ be the unitary matrix defined by

$$U = (2P - I)(2Q - I).$$

That is, U is the product of the reflections through the column spaces of M and N. The *vertex-face (quantum) walk* on X, given an initial state $|\psi\rangle \in \mathbb{C}^{\mathcal{A}}$, is given by the sequence $(U^t |\psi\rangle)_{t \in \mathbb{Z}_{\geqslant 0}}$, and U the *transition matrix* of the vertex-face walk on X, or 'transition matrix of X' for short. Note that all of the matrices involved have real entries. The transition matrix for the dual map is given by

$$(2Q - I)(2P - I) = U^T,$$

which is the inverse of U, since $U^* = U^T$. We note that we have made an arbitrary decision, following Zhan [31], to use the clockwise flags; one can derive a more formal correspondence between the use of clockwise and anticlockwise flag using equation (5).

For the map X_2 whose arcs are shown in Figure 4, we can compute that

$$U = I_2 \otimes \begin{bmatrix} 0\ 1 \\ 1\ 0 \end{bmatrix}$$

and thus $U^2 = I$; in this case the vertex-face walk will alternate between two states. Various characterisations of maps for which the transition matrix U satisfies $U^2 = I$ are given in Lemma 7.2.

To give a more visual example, we consider the Heawood graph embedded on the torus, whose dual is K_7. See Figure 6. Let $|\psi\rangle$ be the state consisting of the uniform superposition of the out-going arcs of vertex 6; that is $|\psi\rangle = \widehat{N} \mathbf{e}_6$. Similarly, let $|\phi\rangle := \widehat{N} \mathbf{e}_4$ be the state consisting of the uniform superposition of the out-going arcs of vertex 4. The probability of measuring at $|\phi\rangle$ at time t with initial state $|\psi\rangle$ is given by $|\langle \phi | U^t | \psi \rangle|^2$. The plot on the right side of Figure 6 shows this probability for $t = 0, \ldots, 49$.

The following result about the 1 and (-1)-eigenspaces of U is due to [22] for general quantum walks and appears as [31, Theorems 3.1, 3.3] for vertex-face walks. Recall that $C = N^T M$.

THEOREM 3.1. [31] *Let U be the transition matrix for the vertex-face walk of an orientable map X.*

(i) *The 1-eigenspace of U is*

$$(\operatorname{col}(M) \cap \operatorname{col}(N)) \oplus (\ker(M^T) \cap \ker(N^T))$$

and has dimension $|E| + 2g$. The first subspace in this direct sum is

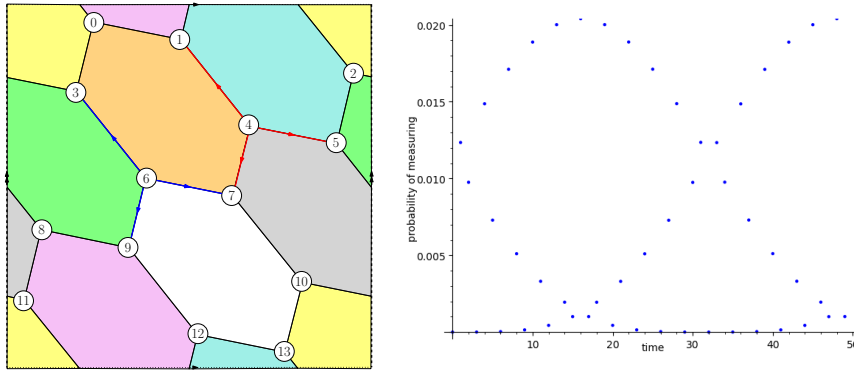$$\operatorname{col}(M) \cap \operatorname{col}(N) = \operatorname{span}\{\mathbf{1}\}.$$

FIGURE 6. An embedding of the Heawood graph on the torus with the out-arcs at vertices 6 and 4 distinguished.

(ii) *The* (-1)-*eigenspace of* U *is*

$$(\operatorname{col}(M) \cap \ker(N^T)) \oplus (\ker(M^T) \cap \operatorname{col}(N))$$

and has dimension $|V| + |F| - 2\operatorname{rk}(C)$. $\qquad\square$

We see that the all-ones vector $\mathbf{1}$ is always in the 1-eigenspace of U, so the 1-eigenspace is non-trivial. Note that the expression for the dimension of the (-1)-eigenspace is always nonnegative. This space is trivial only if the number of vertices of the map equals the number of faces:

COROLLARY 3.2. *If* -1 *is not an eigenvalue of* U, *then* $|V| = |F|$.

Proof. If -1 is not an eigenvalue of U, then the dimension of its (-1)-'eigenspace' is 0. By Theorem 3.1(ii), this implies that

$$|V| + |F| = 2\operatorname{rk}(C).$$

Since the rank of C is at most $\min(|V|, |F|)$, we must have $|V| = |F|$. $\qquad\square$

As U is real and unitary, eigenvalues other than ± 1 come in conjugate pairs and lie on the unit circle. (Theorem 3.1 implies that there are $\operatorname{rk}(C) - 1$ such pairs, with multiplicity.) The following result describes how these eigenvalues arise from a smaller matrix whose rows and columns are indexed by the vertex set: $\widehat{C}\widehat{C}^T = \widehat{N}^T P \widehat{N}$, where $\widehat{C} = \widehat{N}^T \widehat{M}$. As shown in [31], the eigenvalues of U can be expressed in terms of the eigenvalues of this matrix. To better facilitate our results, we give a restatement of their result as a decomposition of the space $\mathbb{C}^{\mathcal{A}}$ into root spaces, along with the minimal polynomials of U over each root space, each of which has degree at most 2.

THEOREM 3.3. [31] *Let* $\{\mathbf{v}_i\}_{i=1}^{|V|} \subset \mathbb{C}^V$ *be an orthogonal eigenbasis of* $\widehat{C}\widehat{C}^T$, *with corresponding eigenvalues* $\hat{\lambda}_1, \ldots, \hat{\lambda}_{|V|}$. *Then* $\mathbb{C}^{\mathcal{A}}$ *can be decomposed into a direct sum of orthogonal subspaces as follows:*

$$\mathbb{C}^{\mathcal{A}} = \mathcal{K} \oplus \mathcal{W} \oplus \bigoplus_{i:\hat{\lambda}_i \notin \{0,1\}} \mathcal{J}_i,$$

where $\mathcal{K}$ *is the* 1-*eigenspace and* $\mathcal{W}$ *the* (-1)-*eigenspace of* U, *and where*

$$\mathcal{J}_i = \operatorname{span}\{\widehat{N}\mathbf{v}_i, P\widehat{N}\mathbf{v}_i\}, \quad i = 1, \ldots, |V|.$$

If $\hat{\lambda}_i \neq 0, 1$, *the minimal polynomial of* U *over* $\mathcal{J}_i$ *is given by*

$$p_i(t) = t^2 - (4\hat{\lambda}_i - 2)t + 1. \qquad\square$$

Note that if X is a type (k, d) map (i.e. every vertex has degree d and every face has degree k), then $\widehat{C}\widehat{C}^T = CC^T/(kd)$. As an example, let X be the 2×3 grid embedded in the torus. For this map, the eigenvalues of CC^T are as follows: $\lambda_1 = \lambda_2 = \lambda_3 = 0$, $\lambda_4 = \lambda_5 = 4$, and $\lambda_6 = 16$. The eigenvalues of $\widehat{C}\widehat{C}^T$ are then given by $\hat{\lambda}_i = \lambda_i/16$ for all i. Then $\lambda_4, \lambda_5 \in (0, 1)$, so that

$$\mathbb{C}^{\mathcal{A}} = \mathcal{K} \oplus \mathcal{W} \oplus \mathcal{J}_4 \oplus \mathcal{J}_5,$$

where the 1-eigenspace $\mathcal{K}$ of U has dimension 14 and the (-1)-eigenspace $\mathcal{W}$ has dimension 6. The spaces $\mathcal{J}_4$ and $\mathcal{J}_5$ are two-dimensional subspaces over which U has minimal polynomial

$$p_4(t) = p_5(t) = t^2 + t + 1.$$

Indeed, the dimensions of these subspaces sum to $|\mathcal{A}| = 24$.

Recall that if a type (k, d) map has incidence multiplicity α, then, whenever a vertex v is incident to a face f, that vertex v is traversed exactly α times by the facial walk of f. In the following lemma, we generalize Lemma 2.3 from [31] from circular embeddings to type (k, d) maps of any incidence multiplicity.

LEMMA 3.4. *If X is a type (k, d) map with an incidence multiplicity α, then every diagonal entry of U is equal to*

$$\frac{4\alpha}{kd} - \frac{2}{k} - \frac{2}{d} + 1.$$

Moreover,

$$\text{tr}(U) = \frac{4\alpha|V|}{k} - 2|F| - 2|V| + |\mathcal{A}|.$$

Proof. We have $Q = \frac{1}{d}NN^T$ and $P = \frac{1}{k}MM^T$ because X has type (k, d). It is not difficult to see that for all $a, b \in \mathcal{A}$:

$$Q_{a,b} = \begin{cases} \frac{1}{d} & \text{if } v(a) = v(b); \\ 0 & \text{otherwise,} \end{cases} \quad \text{and} \quad P_{a,b} = \begin{cases} \frac{1}{k} & \text{if } f(a) = f(b); \\ 0 & \text{otherwise,} \end{cases}$$

where $v(c)$ and $f(c)$ are respectively the vertex and face incident with the arc c. This implies that

$$(PQ)_{a,a} = \sum_{c \in \mathcal{A}} P_{a,c}Q_{c,a} = \frac{\#\text{arcs incident to both } v(a) \text{ and } f(a)}{kd} = \frac{\alpha}{kd}.$$

Since U can be written as

$$U = 4PQ - 2P - 2Q + I,$$

we find that for $a \in \mathcal{A}$:

$$U_{a,a} = \frac{4\alpha}{kd} - \frac{2}{k} - \frac{2}{d} + 1$$

and then

$$\text{tr}(U) = |\mathcal{A}| \cdot U_{a,a} = \frac{4\alpha|V|}{k} - 2|F| - 2|V| + |\mathcal{A}|,$$

by using that $|\mathcal{A}| = |F| \cdot k = |V| \cdot d$. $\square$

4. Perfect state transfer

In this section, we define perfect state transfer for the vertex-face walk and give necessary and sufficient conditions for it to occur. In order to do this, we first work in a more general setting for discrete-time quantum walks and define an auxiliary sequence of matrices describing the walk, which satisfies a Chebyshev recurrence. Specifying to the vertex-face walk, we culminate in some fundamental properties in Theorem 4.5.

In the two-reflection model of a discrete-time quantum walk, the transition matrix U is of the form

$$U = (2WW^* - I)(2VV^* - I),$$

where $W \in \mathbb{C}^{k,n}$ and $V \in \mathbb{C}^{k,m}$ are matrices with orthonormal columns (i.e. $W^*W = I_n$ and $V^*V = I_m$).

We now define an auxiliary sequence of matrices corresponding to U, which will allow us to work with Hermitian matrices. For all $t \in \mathbb{Z}_{\geqslant 0}$, let

$$B_t := V^*U^tV.$$

We may view B_t as the restriction of U^t to the column space of V. Whereas U is not usually Hermitian, the matrix B_t is Hermitian for all t: $B_0 = I$ and, since $(2VV^* - I)$ acts as the identity on V, for $t > 0$, we can write

$$B_t = V^* \left((2WW^* - I)(2VV^* - I)\right)^t V$$
$$= V^* \left((2WW^* - I)(2VV^* - I)\right)^{t-1} (2WW^* - I)V,$$

which is clearly Hermitian. In the following theorem, we show that the sequence $\{B_t\}_{t=0}^{\infty}$ satisfies the same recurrence as the Chebyshev polynomials of the first kind; for more background on Chebyshev polynomials, we refer to [26].

THEOREM 4.1. *For all $t \in \mathbb{Z}_{\geqslant 0}$, we have*

$$B_t = T_t(B_1),$$

where T_t is the t-th Chebyshev polynomial of the first kind.

Proof. Since $B_0 = I$, it suffices to show that B_t satisfies the recursion

$$B_{t+1} = 2B_tB_1 - B_{t-1}.$$

In order to do so, define $D_t = V^*U^tWW^*V$, so that $D_0 = V^*WW^*V$. We claim that B_t and D_t satisfy

$$(6) \qquad \begin{cases} B_{t+1} = 2D_t - B_t \\ D_{t+1} = 2B_{t+1}D_0 - D_t \end{cases}$$

for all $t \geqslant 1$. By applying the claim three times, we find

$$\begin{aligned} B_{t+1} &= 2D_t - B_t \\ &= 4B_tD_0 - 2D_{t-1} - B_t \\ &= 4B_tD_0 - (B_t + B_{t-1}) - B_t \\ &= 2B_t(2D_0 - I) - B_{t-1} \\ &= 2B_tB_1 - B_{t-1}, \end{aligned}$$

for all $t \geqslant 1$, as desired. It remains to prove (6). Since $(2VV^* - I)V = V$, we find that

$$B_{t+1} = V^*U^t(2WW^* - I)V = 2V^*U^tWW^*V - V^*U^tV = 2D_t - B_t.$$

Finally, we have

$$\begin{aligned}
D_{t+1} &= V^*U^t(2WW^* - I)(2VV^* - I)WW^*V \\
&= 2V^*U^t(2WW^* - I)VV^*WW^*V - V^*U^t(2WW^* - I)WW^*V \\
&= 2V^*U^{t+1}VV^*WW^*V - V^*U^tWW^*V \\
&= 2B_{t+1}V^*WW^*V - D_t \\
&= 2B_{t+1}D_0 - D_t,
\end{aligned}$$

where for the third equality, we used for the first term that $V = (2VV^* - I)V$, and for the second term that $(2WW^* - I)W = W$. $\qquad\square$

Denote by $\mathbf{e}_u$ the u-th standard basis vector, so that $V\mathbf{e}_u$ is the u-th column of V. We now use the recurrence to show symmetry for state transfer from $V\mathbf{e}_u$ to $V\mathbf{e}_v$ and $V\mathbf{e}_v$ to $V\mathbf{e}_u$.

LEMMA 4.2. *We have $U^\tau V\mathbf{e}_u = V\mathbf{e}_v$ if and only if $B_\tau(u,v) = B_\tau(v,u) = 1$.*

Proof. If $U^\tau V\mathbf{e}_u = V\mathbf{e}_v$, then by multiplying both sides by $\mathbf{e}_v^*V^*$ on the left, we obtain

$$B_\tau(u,v) = B_\tau(v,u) = \mathbf{e}_v^*B_\tau\mathbf{e}_u = 1$$

since B_τ is Hermitian. Conversely, if $\mathbf{e}_v^*B_\tau\mathbf{e}_u = 1$, then

$$\langle V\mathbf{e}_v, U^\tau V\mathbf{e}_u\rangle = 1,$$

and as both $V\mathbf{e}_v$ and $U^\tau V\mathbf{e}_u$ have unit length, this implies $U^\tau V\mathbf{e}_u = V\mathbf{e}_v$. $\qquad\square$

The matrices B_i allow us to connect when the quantum walk takes a specific uniform superposition at u to another vertex v with an algebraic property of the graph, which we will now define. Let M be a Hermitian matrix with rows and columns indexed by a set Ω, and let

$$M = \sum_{r=0}^{d}\theta_r E_r$$

be the spectral decomposition of M. Then $u, v \in \Omega$ are said to be *strongly cospectral with respect to M* if

$$E_r\mathbf{e}_v = \pm E_r\mathbf{e}_u$$

for all $r = 0, \ldots, d$. Strongly cospectral vertices have been previously studied in the context of continuous-time quantum walks, where M is the adjacency matrix of a graph, see [3]. We obtain the following directly from Theorem 4.1.

COROLLARY 4.3. *Let $u, v \in \{1, \ldots, m\}$. Then the following hold:*
  (i) *$U^\tau V\mathbf{e}_u = V\mathbf{e}_v$ if and only if $U^\tau V\mathbf{e}_v = V\mathbf{e}_u$*
  (ii) *If $U^\tau V\mathbf{e}_u = V\mathbf{e}_v$, then u and v are strongly cospectral with respect to B_d for all divisors d of τ.*

Proof. Part (i) follows from Lemma 4.2 and the fact that B_t is symmetric for all t.

For (ii), let d be any positive integer that divides τ. Let the following be the spectral decomposition of B_d:

$$B_d = \sum_\theta \theta F_\theta.$$

By Theorem 4.1 and by the properties of T_t under composition (see [26, Exercise 1.1.6]), that

$$B_\tau = T_\tau(B_1) = T_\ell(T_d(B_1)) = T_\ell(B_d),$$

where $\ell = \tau/d$. Since $B_\tau \mathbf{e}_u = \mathbf{e}_v$, we have for every eigenvalue σ of B_d:

$$F_\sigma \mathbf{e}_v = F_\sigma B_\tau \mathbf{e}_u = F_\sigma T_\ell(B_d)\mathbf{e}_u = F_\sigma \sum_\theta T_\ell(\theta)F_\theta \mathbf{e}_u = T_\ell(\sigma)F_\sigma \mathbf{e}_u.$$

Repeating the argument for $F_\sigma \mathbf{e}_u$, since $B_\tau \mathbf{e}_v = \mathbf{e}_u$, we see that $F_\sigma \mathbf{e}_u = T_\ell(\sigma)F_\sigma \mathbf{e}_v$. Thus, we find that

$$F_\sigma \mathbf{e}_u = T_\ell(\sigma)F_\sigma \mathbf{e}_v = T_\ell(\sigma)^2 F_\sigma \mathbf{e}_u$$

and thus $T_\ell(\sigma) \in \{\pm 1\}$ unless $F_\sigma \mathbf{e}_u = F_\sigma \mathbf{e}_v = 0$, and the result follows. $\qquad\square$

Now we will apply this idea to the vertex-face walk. Recall that for a map X, the transition matrix U of X for the vertex-face walk is defined by

$$U = (2P - I)(2Q - I),$$

where $P = \widehat{M}\widehat{M}^T$ and $Q = \widehat{N}\widehat{N}^T$ are the projectors onto the column spaces of M and N respectively, and $\widehat{M}$ and $\widehat{N}$ are the normalized arc-face and arc-vertex incidence matrices. When we consider the evolution of a quantum system, we usually take the initial state to be a uniform superposition of all arcs incident to some vertex u; in particular, we consider the state $\widehat{N}\mathbf{e}_u$, where $\mathbf{e}_u \in \mathbb{C}^V$ is the elementary basis vector indexed by u.

For vertices $u, v \in V$, if

$$U^\tau \widehat{N}\mathbf{e}_u = \mathbf{x}, \tag{7}$$

where $\mathbf{x} \in \mathbb{C}^{\mathcal{A}}$ is a unit length vector that satisfies $\widehat{N}\mathbf{e}_w \circ \mathbf{x} = 0$ for all $w \neq v$ (i.e. $\mathbf{x}$ is any superposition of the arcs incident to v), then, if u, v are distinct, we say that there is *perfect state transfer from u to v at time $\tau \in \mathbb{Z}_{>0}$* and if $u = v$, we say that X is *periodic at the vertex u* at time τ. For convenience, we will write uv-*PST* for perfect state transfer from u to v.

By the following lemma, we can simplify the expression in (7) for such maps, using the same ideas as [17, Lemma 3.2.1] for the arc-reversal Grover walk on d-regular graphs. Note that, in the following lemma, the underlying graph is not necessarily d-regular, but the two involved vertices must have the same degree.

LEMMA 4.4. *Let X be a map and u, v be vertices of X with degree d. Then there is uv-PST at time τ if and only if*

$$U^\tau \widehat{N}\mathbf{e}_u = \widehat{N}\mathbf{e}_v. \tag{8}$$

Proof. It is clear that if (8) holds, then there is uv-PST at time τ by definition. For the converse, suppose that there is uv-PST at time τ, so that (7) holds for some appropriate $\mathbf{x}$. Note that $\widehat{N}\mathbf{e}_u = \frac{1}{\sqrt{d}}N\mathbf{e}_u$ and that $\mathbf{1}_{\mathcal{A}}$ is an eigenvector of U^T with eigenvalue 1, where the latter is a consequence of Theorem 3.1, applied to the transition matrix U^T of the dual map. We have

$$\sqrt{d} = \langle \mathbf{1}_{\mathcal{A}}, \widehat{N}\mathbf{e}_u \rangle = \langle (U^T)^\tau \mathbf{1}_{\mathcal{A}}, \widehat{N}\mathbf{e}_u \rangle = \langle \mathbf{1}_{\mathcal{A}}, U^\tau \widehat{N}\mathbf{e}_u \rangle = \langle \mathbf{1}_{\mathcal{A}}, \mathbf{x} \rangle.$$

Since $\mathbf{x}$ takes non-zero entries only on the arcs incident with v, we have that $\langle \mathbf{1}_{\mathcal{A}}, \mathbf{x} \rangle = \langle N\mathbf{e}_v, \mathbf{x} \rangle$, whence we obtain that $\sqrt{d} = \sqrt{d}\langle \widehat{N}\mathbf{e}_v, \mathbf{x} \rangle$. Since both $\widehat{N}\mathbf{e}_v$ and $\mathbf{x}$ have length 1, the equality $\langle \widehat{N}\mathbf{e}_v, \mathbf{x} \rangle = 1$ implies that $\mathbf{x} = \widehat{N}\mathbf{e}_v$. $\qquad\square$

We note that, in the general case, there can only be uv-PST if the degree of v is at least the degree of u; in the proof of Lemma 4.4, the general case yields

$$\sqrt{d(u)} = \sqrt{d(v)}\langle \widehat{N}\mathbf{e}_v, \mathbf{x} \rangle \leqslant \sqrt{d(v)}$$

by Cauchy-Schwarz. We will restrict our attention to perfect state transfer between vertices of equal degree and we can take (8) to be the definition of uv-PST at time τ.

For periodicity at a vertex u, (8) (with $u = v$) is equivalent to the original definition for any map, by Lemma 4.4.

As in the general case, we will consider, for $t \in \mathbb{Z}_{\geqslant 0}$, the matrix

$$B_t = \widehat{N}^T U^t \widehat{N}.$$

It follows directly from Lemmas 4.2 and 4.4 that there is uv-PST at time τ if and only if

$$B_\tau(u, v) = B_\tau(v, u) = 1,$$

and there is periodicity at u at time τ if and only if $B_\tau(u, u) = 1$.

Though B_t is not, in general, a stochastic matrix, we note that for all $t \in \mathbb{Z}_{\geqslant 0}$, the vector $\mathbf{w} = (\sqrt{d(v)})_v$ is an eigenvector for B_t with eigenvalue 1. In particular, if the graph underlying the map is d-regular, every row of B_t sums to 1. In this setting, we have that $B_0 = I$, $B_1 = 2\widehat{C}\widehat{C}^T - I$, and $B_t = T_t(B_1)$ where T_t is the t-th Chebyshev polynomial of the first kind, by Theorem 4.1.

We now apply our results from the general setting and we establish some fundamental properties of perfect state transfer in the vertex-face walk.

THEOREM 4.5. *Consider the vertex-face quantum walk on a map X, and let $u, v \in V(X)$ be distinct vertices of X. Assume that there is uv-PST at time $\tau \in \mathbb{Z}_{>0}$. Then*

  (i) *there is vu-PST at time τ;*
 (ii) *there is periodicity at both u and v at time 2τ;*
(iii) *there does not exist a vertex w, distinct from u and v, such that there is uw-PST at any time; and*
 (iv) *u and v are strongly cospectral with respect to B_d for all divisors d of τ.*

Proof. Clearly, (ii) follows directly from (i). The property (i) follows from Lemma 4.2 and the fact that B_τ is symmetric. For (iii), assume that τ is the smallest time at which there is uv-PST. If there is some $w \neq u, v$ for which there is uw-PST at some time τ', where τ' is also minimal, then there is periodicity at u both at time $2\tau'$ and at time 2τ. The minimality of τ and τ' ensures that both $\tau' < 2\tau$ and $\tau < 2\tau'$. Assume without loss of generality that $\tau' < \tau$. Then there is periodicity at u at time $2(\tau - \tau')$, but

$$2(\tau - \tau') < 2\tau - \tau = \tau,$$

contradicting the minimality of τ.

Part (iv) follows directly from applying Corollary 4.3 with $V = \widehat{N}$ and $W = \widehat{M}$. $\square$

We note that, in particular, if there is uv-PST at any time, the vertices u and v are strongly cospectral with respect to B_1. We remark that the proof of (iv) also implies that $T_d(\sigma) = \pm 1$ if $F_\sigma \mathbf{e}_u \neq 0$, so the *eigenvalue support* of u (and also of v) is the set $\{\pm 1\}$.

5. PERIODIC MAPS

We have seen in Theorem 4.5 of the previous section that uv-PST results in periodicity at u and v at twice the time. Thus if the vertex set partitions into pairs such that perfect state transfer occurs between every pair at time τ, then there is periodicity at every vertex at time 2τ. If the automorphism group of the map acts transitively upon the vertex set and there is uv-PST for some pair of vertices, then there must be perfect state transfer everywhere (see Theorem 5.4). Motivated by this, we will turn our attention to maps where periodicity occurs at every vertex at the same time τ.

Now we will proceed with some formal definitions. Let X be an orientable map. If there is periodicity at every vertex at time τ, i.e. if $U^\tau \widehat{N} = \widehat{N}$, we say that X is

periodic at time τ. Equivalently, X is periodic at time τ if U^τ acts as the identity on
col(N). We call τ the *period* of X if τ is minimal.

In the following theorem, we establish the connection between periodic maps and
those where $U^\tau = I$; we see that, in many cases, periodicity of the map at time τ
implies that $U^\tau = I$, for instance, when τ is even.

THEOREM 5.1. *Let $\tau \in \mathbb{Z}_{>0}$. The transition matrix satisfies $U^\tau = I$ if and only if the
map is periodic at time τ and at least one of the following is satisfied:*

   (a) *τ is even, or*
   (b) *$|V| = |F|$.*

Further, if the map is periodic at time τ, then $U^{2\tau} = I$.

Proof. Define
$$\tilde{U} := U^\tau(2Q - I) = ((2P - I)(2Q - I))^{\tau-1}(2P - I),$$
so that also $U^\tau = \tilde{U}(2Q - I)$. We see that $U^\tau = I$ if and only if $\tilde{U} = 2Q - I$. Moreover,
as $\tilde{U}$ is both unitary and symmetric, it is an involution. In particular, both $\tilde{U}$ and
$2Q - I$ are symmetric with eigenvalues in $\{-1, 1\}$; we can conclude that

(9) $\qquad U^\tau = I \quad \Longleftrightarrow \quad \tilde{U}$ and $2Q - I$ have the same 1-eigenspace.

Now assume that the map is periodic at time $\tau \in \mathbb{Z}_{>0}$. Then
$$\widehat{N} = U^\tau\widehat{N} = \tilde{U}(2Q - I)\widehat{N} = \tilde{U}\widehat{N},$$
so the 1-eigenspace of $\tilde{U}$ contains col(N), which is the 1-eigenspace of $2Q - I$. By (9),
it is now sufficient to show that the multiplicity of the eigenvalue 1 is the same for $\tilde{U}$
and $2Q - I$. Equivalently, we can show that these matrices have equal trace. By using
the cyclic property of the trace, and the fact that $2P - I$ and $2Q - I$ are involutions,
the trace of $\tilde{U}$ can be reduced as follows:
$$\operatorname{tr}(\tilde{U}) = \operatorname{tr}\left[((2P - I)(2Q - I))^{\tau-1}(2P - I)\right]$$
$$= \operatorname{tr}\left[(2Q - I)((2P - I)(2Q - I))^{\tau-2}\right]$$
$$\vdots$$
$$= \begin{cases} \operatorname{tr}(2Q - I) & \text{if } \tau \text{ even;} \\ \operatorname{tr}(2P - I) & \text{if } \tau \text{ odd.} \end{cases}$$

This proves that $U^\tau = I$ if τ is even, or if τ is odd and $\operatorname{tr}(2P - I) = \operatorname{tr}(2Q - I)$. The
latter happens exactly if P and Q have equal rank, i.e. if $|F| = |V|$.

Conversely, assume that $U^\tau = I$. Then the map is certainly periodic at time τ.
Moreover, $\tilde{U} = 2Q - I$, so if τ is odd, then
$$\operatorname{tr}(2Q - I) = \operatorname{tr}(\tilde{U}) = \operatorname{tr}(2P - I),$$
as we saw above. Hence $|V| = |F|$.

Regardless of the parity of τ, periodicity of the map at time τ certainly implies
that $U^{2\tau} = I$, since there is also periodicity at time 2τ. $\qquad\square$

An example for when periodicity of the map at time τ does not imply $U^\tau = I$ is any
map with one vertex and more than one face. For such a map, $N = \mathbf{1}_\mathcal{A}$, meaning that
$U\widehat{N} = \widehat{N}$, so the map is periodic at time $\tau = 1$. But since $|V| < |F|$, Theorem 5.1
implies that $U \neq I$. Nevertheless, this example leads to the following corollary for
maps with a single vertex or face.

COROLLARY 5.2. *For any map with a single vertex or a single face, $U^2 = I$.*

Proof. If the map has a single vertex, then the map is periodic at time 1. If it has a single face, the dual map is periodic at time 1. In either case, $U^2 = I$ by Theorem 5.1. $\square$

For example, any tree embedded in the plane has a single face, so its transition matrix will satisfy $U^2 = I$. It is natural to ask if perfect state transfer can occur at time 1 in trees; Proposition 5.5 will imply that K_2 is the only tree that admits this.

Corollary 5.2 gives a source for generating examples of maps with periodicity at time $\tau = 1$, where $U^\tau \neq I$. We give an example of this, namely the duals of dipoles with a single face, in Section 6.1. We can ask if such maps also exist for $\tau > 1$. Necessarily, for these maps, τ must be odd and $|V| \neq |F|$ by Theorem 5.1. More specifically, the lemma below implies that such maps must satisfy $|V| < |F|$:

LEMMA 5.3. *Let X be a map.*

(i) *Let $\tau > 0$ be odd. The map X is periodic at time τ if and only if*

$$\operatorname{col}\left(U^{\frac{\tau+1}{2}} \widehat{N}\right) \subseteq \operatorname{col}(\widehat{M}).$$

In particular, if X is periodic at time τ, then $|V| \leqslant |F|$.

(ii) *The map X is periodic at time 1 if and only if $|V| = 1$.*

Proof. For part (i), if X is periodic at time τ, then $U^{2\tau} = I$ by Theorem 5.1, so we have that U^τ is an involution and thus $U^\tau = (U^T)^\tau$. Thus, the periodicity implies that $(U^T)^\tau \widehat{N} = \widehat{N}$ and we obtain that

$$(U^T)^{\frac{\tau-1}{2}} \widehat{N} = U^{\frac{\tau+1}{2}} \widehat{N}$$

by multiplying by $U^{\frac{\tau+1}{2}}$ on both sides. Since $\widehat{N} = (2Q-I)\widehat{N}$ and $(2P-I)U^t(2Q-I) = (U^T)^{t-1}$, we can write

$$(2P - I)U^{\frac{\tau+1}{2}} \widehat{N} = (U^T)^{\frac{\tau-1}{2}} \widehat{N} = U^{\frac{\tau+1}{2}} \widehat{N}.$$

Thus $U^{\frac{\tau+1}{2}} \widehat{N}$ is invariant under $2P - I$, so the columns of $U^{\frac{\tau+1}{2}} \widehat{N}$ are in $\operatorname{col}(M)$. In particular, since multiplying by $U^{\frac{\tau+1}{2}}$ preserves the orthonormality of the columns of $\widehat{N}$:

$$|V| = \dim(\operatorname{col}(\widehat{N})) \leqslant \dim(\operatorname{col}(\widehat{M})) = |F|.$$

For part (ii), assume that $U\widehat{N} = \widehat{N}$. Then $\operatorname{col}(\widehat{N}) \subseteq \operatorname{col}(\widehat{M})$ by Lemma 5.3, which implies that

$$\operatorname{col}(\widehat{N}) = \operatorname{col}(\widehat{N}) \cap \operatorname{col}(\widehat{M}) = \operatorname{span}\{\mathbf{1}\}$$

by Theorem 3.1. Hence $|V| = 1$. The other direction was discussed above this lemma. $\square$

In Section 6.2, we give for any $\tau > 0$ a map with $|V| = \tau = |F|$ that satisfies $U^\tau = I$. We then show that, given any one of those maps, we can add a few edges in a way that retains the periodicity at time τ. The newly obtained map has the same number of vertices, but the number of faces has increased. Hence by Theorem 5.1, if τ is odd, $U^\tau \neq I$. In this way, we show in Lemma 6.6 that, for all odd τ, there exists a map that is periodic at time τ such that $U^\tau \neq I$. This shows that the statement of Theorem 5.1 is best possible. The following result relates periodic maps to perfect state transfer.

THEOREM 5.4. *Assume that X is a map such that the automorphism group of X acts transitively on the set of vertices V. Let u and v be vertices of X. The following are true.*

(i) *If there is uv-PST at time τ, then for any vertex x there is a unique vertex y such that there is xy-PST at time τ. Moreover, $U^{2\tau} = I$.*

(ii) *If there is periodicity at u at time τ, then the map is periodic at time τ.*

Proof. For (i), consider any automorphism π of X, and write $\pi_{\mathcal{A}}$ and π_V for the permutation matrices that correspond to the action of π on the sets of arcs and vertices respectively. By Proposition 2.1, we know that $\pi_{\mathcal{A}}\widehat{N} = \widehat{N}\pi_V$ and $\pi_{\mathcal{A}}\widehat{M} = \widehat{M}\pi_F$. From this, we deduce that $\pi_{\mathcal{A}}$ commutes with both P and Q, and hence also with U. This implies that

$$\pi_V^T B_\tau \pi_V = \widehat{N}^T \pi_{\mathcal{A}}^T U^\tau \pi_{\mathcal{A}} \widehat{N} = \widehat{N}^T U^\tau \widehat{N} = B_\tau.$$

Then if u (resp. v) is mapped to the vertex x (resp. y) under π, we have

$$\mathbf{e}_x^T B_\tau \mathbf{e}_y = \mathbf{e}_u^T \pi_V^T B_\tau \pi_V \mathbf{e}_v = \mathbf{e}_u^T B_\tau \mathbf{e}_u = 1,$$

meaning that there is xy-PST at time τ by Lemma 4.2 (and yx-PST by Theorem 4.5(i)). Since the action of the automorphism group is transitive on V, any vertex w is the image of u under the action of some automorphism, so $|V|$ can be partitioned into pairs of vertices that admit perfect state transfer to each other at time τ. Theorem 4.5(ii) then implies that the map is periodic at time 2τ, so $U^{2\tau} = I$ by Theorem 5.1. Property (ii) is similar to (i): if there is periodicity at one vertex, there must be periodicity at every vertex, so the map is periodic. $\square$

By Theorem 5.4(i), if the automorphism group of a map X acts transitively on the vertex set V, then uv-PST at time 1 implies $U^2 = I$. There are many examples of orientably-regular maps that satisfy the property $U^2 = I$, as can be seen from our computations in Section 8, and we give equivalent characterisations of this property in Lemma 7.2. Conversely, we might ask when there can be uv-PST at time 1 if $U^2 = I$. It turns out that this property only occurs for a small family of maps:

PROPOSITION 5.5. *Let X be a map for which the transition matrix U satisfies $U^2 = I$, and let u and v be distinct vertices of equal degree. Then there is uv-PST at time 1 if and only if $V = \{u, v\}$.*

Proof. Assume first that $V = \{u, v\}$. Then X is an embedding of a d-regular graph, where d is the degree of u and v. For such a map, as $U^2 = I$, we find by part (iv) of Lemma 7.2 that

$$\widehat{C}\widehat{C}^T = \frac{d}{|\mathcal{A}|} J_{V \times V} = \frac{1}{|V|} J_{V \times V}.$$

In this case, $|V| = 2$, so we obtain

$$B_1 = 2\widehat{C}\widehat{C}^T - I = J_{V \times V} - I.$$

Then $B_1(u, v) = 1$, so there is uv-PST at time 1 by Lemma 4.2.

For the other implication, note that since $U^2 = I$, part (iv) of Lemma 7.2 implies that

$$\widehat{C}\widehat{C}^T = \mathbf{x}\mathbf{x}^T,$$

where $\mathbf{x} = |\mathcal{A}|^{-\frac{1}{2}} D^{\frac{1}{2}} \mathbf{1}_V$. In particular, $\mathbf{x}_w \neq 0$ for all $w \in V$. If there is uv-PST at time 1, then $B_1(u, v) = 1$ by Lemma 4.2, so we must have $\mathbf{x}_u \mathbf{x}_v = \frac{1}{2}$. However, $\mathbf{x}$ has norm 1 with entries between 0 and 1, which implies that $\mathbf{x}_u \mathbf{x}_v = \frac{1}{2}$ if and only if $\mathbf{x}_u = \mathbf{x}_v = \frac{1}{\sqrt{2}}$ and $\mathbf{x}_w = 0$ for $w \neq u, v$. We conclude that $V = \{u, v\}$. $\square$

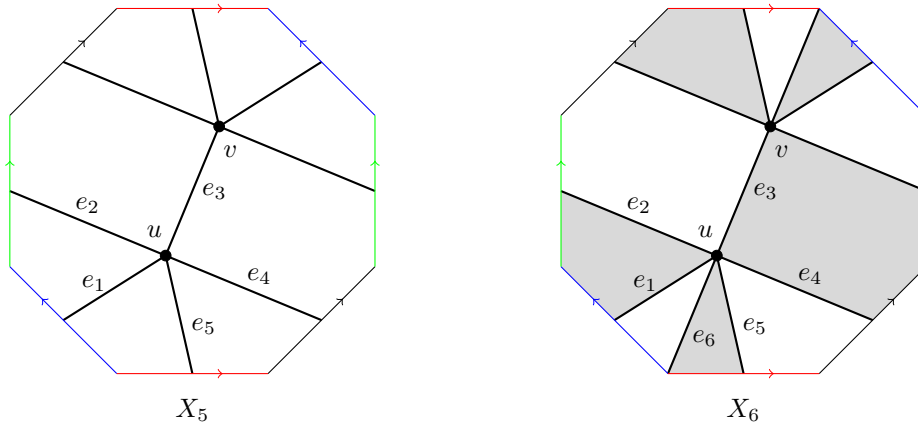The dipoles that we discuss in Section 6.1 are examples of these maps.

FIGURE 7. The maps X_5 and X_6 on the double torus. We can obtain X_6 from X_5 by adding an edge e_6 that passes through the identified corners of the octagon.

6. INFINITE FAMILIES OF EXAMPLES

In this section, we give several infinite families of maps which exhibit perfect state transfer and periodicity. In Section 6.1, we give an infinite family of maps with two vertices which admit perfect state transfer at time 1. In Section 6.2, we give two infinite families of grids which admit perfect state transfer and also a variant family which admits periodicity at every vertex at some time s, but where $U^s \neq I$. The last family shows that, in some sense, the statement of Theorem 5.1 is best possible.

6.1. DIPOLES WITH ONE OR TWO FACES. A *dipole* is a graph with two vertices and no loops. Dipoles encode information in many ways and have been studied in various contexts, see [11]. Here we study a specific rotation system for dipoles, which results in an embedding with either one face or two faces, depending on the parity of the number of edges. Perfect state transfer occurs at time 1 in these embeddings of dipoles; they are maps whose automorphism group acts transitively on the vertex set and thus illustrate Proposition 5.5.

For $n \in \mathbb{Z}_{>0}$, consider the map X_n with two vertices u and v, with edges $e_1, \ldots, e_n$, and rotation system

$$u : (e_1, e_2, \ldots, e_n), \qquad v : (e_1, e_2, \ldots, e_n).$$

That is, every edge is incident to both vertices and the edges appear in the same order around each vertex. Figure 7 depicts X_5 and X_6. Let the arcs of the map be given by a_i and b_i for $i = 1, \ldots, n$, such that each edge e_i is incident to the pair of arcs (a_i, b_i), with a_i and b_i having u and v as their respective tails. In other words, we can write

$$u : (a_1, a_2, \ldots, a_n), \qquad v : (b_1, b_2, \ldots, b_n)$$

for the rotation system with respect to the arcs of the map. If n is odd, the map has a single facial walk given by sequence of arcs

$$(a_n, b_{n-1}, a_{n-2}, b_{n-3}, \ldots, a_1, b_n, a_{n-1}, b_{n-2}, a_{n-3}, \ldots, b_1).$$

If n is even on the other hand, the map has two facial walks given by the sequences

$$(a_n, b_{n-1}, a_{n-2}, b_{n-3}, \ldots, b_1) \qquad \text{and} \qquad (b_n, a_{n-1}, b_{n-2}, a_{n-3}, \ldots, a_1).$$
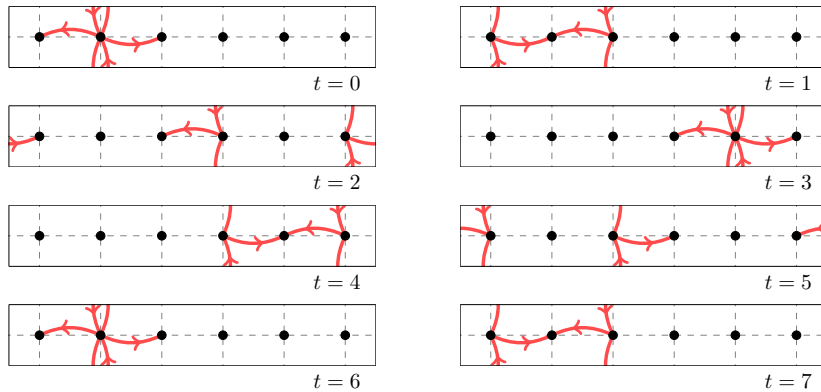
FIGURE 8. Evolution of the walk on the $(1,6)$-grid, with perfect state transfer at time 3 and periodicity at time 6. The graphs are drawn on the cut-open torus, where the opposite sides are identified; for visual simplicity, we have omitted the labels on the boundary of the torus. At every step, the arcs with a non-zero amplitude are shown.

Thus the genus of the map is

$$g = \begin{cases} \frac{n-1}{2}, & \text{if } n \text{ is odd;} \\ \frac{n-2}{2}, & \text{if } n \text{ is even.} \end{cases}$$

THEOREM 6.1. *There is uv-PST occurring at time 1 in X_n, for all $n \geqslant 2$.*

Proof. The vertex-face incidence matrix C satisfies

$$C = \begin{bmatrix} n \\ n \end{bmatrix} \quad \text{or} \quad C = \frac{1}{2} \begin{bmatrix} n & n \\ n & n \end{bmatrix},$$

when n is odd or even, respectively. In either case, we obtain that $B_1 = 2\widehat{C}\widehat{C}^T - I_2 = J_2 - I_2$ (where J_2 is the 2×2 all-ones matrix), and the result follows by Lemma 4.2. $\square$

6.2. TOROIDAL GRIDS. In [24, 12, 1], quantum search is studied on the toriodal grid. Zhan generalized the unitary operator without the query matrix to the vertex-face walk, in the two-reflection model, and details the connection with these search algorithms in [31, Section 8]. In this section, we find perfect state transfer and periodicity in some toroidal grids.

Figure 8 shows the evolution of the walk on the 1×6 grid embedded on the torus, starting at the uniform superposition of a vertex. As is suggested by the figure, perfect state transfer occurs at time $t = 3$. We will now proceed by giving a rigorous definition of the toroidal grids before proving our main theorems establishing the perfect state transfer in the toroidal $(1, m)$-grids for m even and in the $(2, m)$-grids for m odd. We also alter the $(1, m)$-grids to give an infinite family of examples which admit periodicity at every vertex at time time s but where $U^s \neq I$.

The *toroidal (n, m)-grid* has vertex set $V = \mathbb{Z}_n \times \mathbb{Z}_m$ and edge set

$$E = \{v_R \mid v \in V\} \cup \{v_D \mid v \in V\}$$

such that for all $(a, b) \in V$:

- the edge $(a, b)_R$ is incident with the vertices $(a, b+1)$ and (a, b);
- the edge $(a, b)_D$ is incident with the vertices $(a+1, b)$ and (a, b).
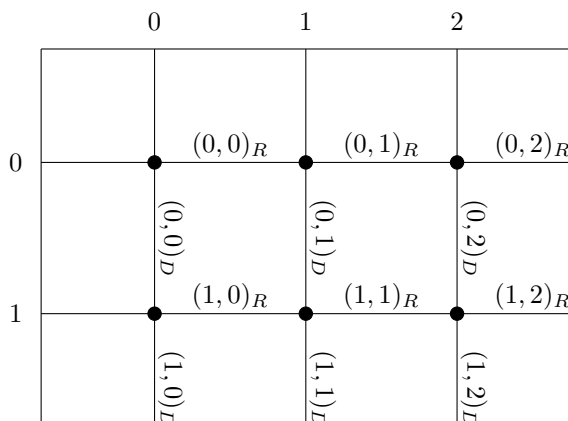
FIGURE 9. The embedding of toroidal $(2,3)$-grid. The vertices are given by the row and column numbers.

For the rotation system, the edges incident with the vertex $(a, b) \in V$ are ordered as follows:

$$(a,b)_R, \ (a,b)_D, \ (a, b-1)_R, \ (a-1, b)_D.$$

The corresponding map has genus 1. For example, in Figure 9, the top left vertex is vertex $(0,0)$ and is incident to $(0,0)_R$ (the edge to its right), to $(0,0)_D$ (the edge downwards from $(0,0)$), as well as $(1,0)_D$ and $(0,2)_R$.

Note that for $n, m \geqslant 3$, the toroidal (n,m)-grid is an embedding of the graph $C_n \square C_m$. For n or m less than 3, the underlying graph has multi-edges and/or loops. It is easy to see that the toroidal (n,m)-grid and (m,n)-grid are isomorphic as maps; to avoid redundancy, we will state our results only for $n \leqslant m$. In the following lemma, we give an expression for the vertex-face incidence matrix of the toroidal (n,m)-grid. Throughout this section, we denote by P_k the cyclic $k \times k$ permutation matrix that maps the standard basis vector $\mathbf{e}_i \in \mathbb{C}^k$ to $\mathbf{e}_{i-1}$, with the index modulo k.

LEMMA 6.2. *The vertex-face incidence matrix C of the toroidal (n,m)-grid can, with an appropriate ordering of the vertices and faces, be written as*

$$C = (P_n + I_n) \otimes (P_m + I_m).$$

Proof. First, assume that $n, m \geqslant 2$. We partition the vertices and faces of X by 'row': that is, we define

$$V_i = \{(i,j) : j \in \mathbb{Z}_m\} \quad \text{and} \quad F_i = \{f_{i,j} : j \in \mathbb{Z}_m\}.$$

Here, the faces are labelled in such a way that every vertex (i,j) in V_i is incident to two elements of F_i (namely $f_{i,j}$ and $f_{i,j-1}$) and two elements of F_{i-1} (namely $f_{i-1,j}$ and $f_{i-1,j-1}$). The submatrix of C corresponding to the vertices of V_i and the faces of F_i is (with an appropriate ordering) given by $P_m + I_m$. The submatrix of C corresponding to V_i and F_{i-1} is also given by $P_m + I_m$. Consequently, it is not difficult to see that

(10) $$C = (P_n + I_n) \otimes (P_m + I_m).$$

If instead $n = 1$ and $m > 1$, then there is only one 'row' of vertices and faces; we find

$$C = 2(P_m + I_m).$$

Similarly, $C = 2(P_n + I_n)$ if $n > 1$ and $m = 1$, and finally $C = [4]$ if $n = m = 1$. These expressions coincide with with (10) (note that $P_1 = [1]$), so that in fact (10) holds for all $n, m \geqslant 1$. $\qquad \square$

In the following lemmas, we look at the structure of the matrices B_t for the toroidal $(1, m)$- and $(2, m)$-grids, in order to prove that perfect state transfer occurs. Note that $P_m^{-t} = (P_m^t)^T$.

LEMMA 6.3. *For the toroidal $(1, m)$-grid, we have*

(11) $$B_t = \frac{1}{2}(P_m^t + P_m^{-t})$$

for all $t \in \mathbb{Z}_{\geqslant 0}$.

Proof. The equation clearly holds for $t = 0$. For $t = 1$, note that by Lemma 6.2:

$$\widehat{C} = \frac{1}{4}C = \frac{1}{2}(P_m + I_m),$$

since the map has type $(4, 4)$. We will show that (11) holds by induction. For $t = 1$, we see that

$$B_1 = 2\widehat{C}\widehat{C}^T - I_m = \frac{1}{2}(P_m + I_m)(P_m + I_m)^T - I_m = \frac{1}{2}(P_m + P_m^{-1}).$$

By Theorem 4.1, B_t satisfies the recurrence of the Chebyshev polynomials of the first kind, and thus

$$
\begin{aligned}
B_{t+1} &= 2B_t B_1 - B_{t-1} \\
&= \frac{1}{2}(P_m^t + P_m^{-t})(P_m + P_m^{-1}) - \frac{1}{2}(P_m^{t-1} + P_m^{-(t-1)}) \\
&= \frac{1}{2}(P_m^{t+1} + P_m^{t-1} + P_m^{-t+1} + P_m^{-t-1}) - \frac{1}{2}(P_m^{t-1} + P_m^{-(t-1)}) \\
&= \frac{1}{2}(P_m^{t+1} + P_m^{-(t+1)}).
\end{aligned}
$$

The result now follows. $\qquad \square$

Another grid that admits perfect state transfer is the $(2, m)$-toroidal grid, for any odd m, as will be a consequence of the next lemma.

LEMMA 6.4. *For the toroidal $(2, m)$-grid, we have*

(12) $$B_t = \frac{1}{4}J_2 \otimes (P_m^t + P_m^{-t} - 2(-1)^t I_m) + (-1)^t I_m \otimes I_m$$

for all $t \in \mathbb{Z}_{\geqslant 0}$.

Proof. We proceed in a similar manner as for the previous lemma. The equation clearly holds for $t = 0$. For $t = 1$, note that

$$\widehat{C} = \frac{1}{4}C = \frac{1}{4}J_2 \otimes (P_m + I_m)$$

by Lemma 6.2. We proceed by induction. Since $J_2 J_2^T = 2J_2$, we find that

$$B_1 = 2\widehat{C}\widehat{C}^T - I_{2m} = \frac{1}{4}J_2 \otimes (P_m + P_m^{-1} + 2I_m) - I_{2m},$$

which coincides with (12). Let $A_t = P_m^t + P_m^{-t} - 2(-1)^t I_m$. Using Theorem 4.1 for the inductive step, we obtain

$$B_{t+1} = 2B_t B_1 - B_{t-1}$$

$$= 2\left(\frac{1}{4}J_2 \otimes A_t + (-1)^t I_{2m}\right)\left(\frac{1}{4}J_2 \otimes A_1 - I_{2m}\right) - \frac{1}{4}J_2 \otimes A_{t-1} - (-1)^{t-1}I_{2m}$$

$$= \frac{1}{8}J_2^2 \otimes A_t A_1 - \frac{1}{2}J_2 \otimes A_t + \frac{1}{2}(-1)^t J_2 \otimes A_1 - 2(-1)^t I_{2m}$$

$$\qquad - \frac{1}{4}J_2 \otimes A_{t-1} - (-1)^{t-1}I_{2m}$$

$$= \frac{1}{4}J_2 \otimes \left(A_t A_1 - 2A_t + 2(-1)^t A_1 - A_{t-1}\right) + (-1)^{t+1}I_{2m}.$$

Since

$$A_t A_1 = (P_m^t + P_m^{-t} - 2(-1)^t I_m)(P_m + P_m^{-1} + 2I_m)$$

$$= P_m^{t+1} + P_m^{t-1} + P_m^{-t+1} + P_m^{-t-1} - 2(-1)^t(P_m + P_m^{-1}) + 2(P_m^t + P_m^{-t}) - 4(-1)^t I_m$$

$$= A_{t+1} + A_{t-1} - 4(-1)^t I_m - 2(-1)^t(A_1 - 2I_m) + 2(A_t + 2(-1)^t I_m) - 4(-1)^t I_m$$

$$= A_{t+1} + A_{t-1} - 2(-1)^t A_1 + 2A_t,$$

we see that $B_{t+1} = \frac{1}{4}J_2 \otimes A_{t+1} + (-1)^{t+1}I_{2m}$, as desired. $\qquad\square$

We now use the form of B_t given by Lemmas 6.3 and 6.4, to obtain our perfect state transfer results on the grids.

THEOREM 6.5.
  (a) *For the toroidal $(1, m)$-grid, the map is periodic at time m. If $m = 2\ell$ is even, there is perfect state transfer from vertex $(0, i)$ to vertex $(0, i + \ell)$ at time ℓ for all $i \in \mathbb{Z}_m$.*
  (b) *For the toroidal $(2, m)$-grid, if m is even, the map is periodic at time m. If m is odd, there is perfect state transfer from vertex $(0, i)$ to vertex $(1, i)$ at time m for all $i \in \mathbb{Z}_m$, and the map is periodic at time $2m$.*

Proof. For part (a), by Lemma 6.3 and the fact that $P_m^m = I$, we have

$$B_m = \frac{1}{2}(P_m^t + P_m^{-t}) = I_m.$$

This is equivalent to the map being periodic at time m. If $m = 2\ell$ is even, then

$$P_m^\ell = P_m^{-\ell} = \begin{bmatrix} 0 & I_\ell \\ I_\ell & 0 \end{bmatrix},$$

which implies that there is perfect state transfer from vertex $(0, i)$ to vertex $(0, i + \ell)$ at time ℓ, by Lemma 4.2.

For part (b), by Lemma 6.4, we have

$$B_m = \frac{1}{4}J_2 \otimes (P_m^m + P_m^{-m} - 2(-1)^m I_m) + (-1)^m I_m \otimes I_m$$

Clearly, if m is even, then $P_m^m + P_m^m - (-1)^m I_m = 0$, so $B_m = I_m \otimes I_m$ and the map is periodic at time m. If m is odd, then

$$B_m = J_2 \otimes I_m - I_m \otimes I_m.$$

This matrix swaps the vertices $(0, i)$ and $(1, i)$ for all $i \in \mathbb{Z}_m$, hence there is perfect state transfer between these pairs of vertices. Finally, $B_{2m} = I_m \otimes I_m$, so the map is periodic at time $2m$. $\qquad\square$
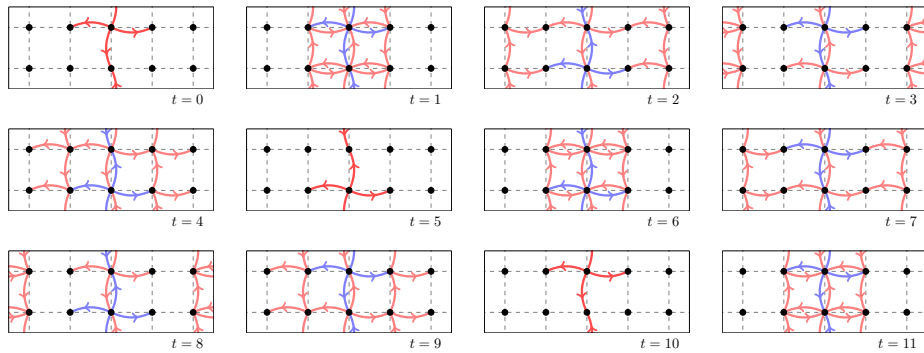
FIGURE 10. The toroidal $(2, 5)$-grid, with perfect state transfer at time 5 and periodicity at time 10. The graphs are drawn on the cut-open torus, where the opposite sides are identified; for visual simplicity, we have omitted the labels on the boundary of the torus. The color (red, blue) represents the sign of the amplitude of an arc (positive, negative, resp.).

Next, we alter the toroidal $(1, m)$-grid to construct an infinite family of maps which have periodicity at every vertex with period m, such that $U^m \neq I$ when m is odd. Figure 11 shows the altered map for the toroidal $(1, 5)$-grid.

LEMMA 6.6. *Let Y_m be the toroidal map obtained from the toroidal $(1, m)$-grid by replacing every non-loop edge by a digon. Then Y_m is periodic with period m. If m is odd, then $U^m \neq I$.*

Proof. By Lemma 6.2, the vertex-face incidence matrix for the toroidal $(1, m)$-grid can be written as
$$C = 2(I_m + P_m),$$
Replacing every non-loop edge of this grid by a digon introduces m new faces of degree 2, each of which is incident to two vertices. Hence the vertex-face incidence matrix of Y_m can be written as
$$C_* = \begin{bmatrix} C & \frac{1}{2}C \end{bmatrix}.$$

The vertices of Y_m have degree 6, the 'original' faces have degree 4, and the newly introduced faces have degree 2. The normalized vertex-face incidence matrix of Y_m can hence be written as
$$\widehat{C}_* = \frac{1}{\sqrt{6}}C_* \begin{bmatrix} \frac{1}{2}I_m & 0 \\ 0 & \frac{1}{\sqrt{2}}I_m \end{bmatrix}$$
$$= \frac{1}{\sqrt{6}} \begin{bmatrix} \frac{1}{2}C & \frac{1}{2\sqrt{2}}C \end{bmatrix}.$$

This implies that
$$\widehat{C}_* \widehat{C}_*^T = \frac{1}{6}\left(\frac{1}{4}CC^T + \frac{1}{8}CC^T\right) = \frac{1}{16}CC^T = \widehat{C}\widehat{C}^T.$$

So Y_m has the same B_t-matrix as the toroidal $(1, m)$-grid, for all t. Since the latter is periodic at time m by Lemma 6.3, the former is as well. Now $|V(X_m)| < |F(Y_m)|$, so for m odd, $U^m \neq I$ by Theorem 5.1. $\square$
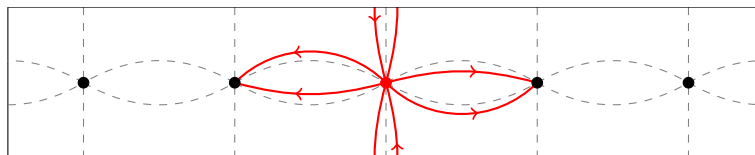
FIGURE 11. The toroidal $(1,5)$-grid with doubled non-loop edges, Y_5, has periodicity at time 5 at every vertex, but $U^5 \neq I$. The graph is drawn on the cut-open torus, where the opposite sides are identified; for visual simplicity, we have omitted the labels on the boundary of the torus.

edges	maps	$\sigma(CC^T) \subset \mathbb{Z}$	periodicity			
			$U = I$	$U^2 = I$	$U^6 = I$	$U^{12} = I$
regular	22320	19226	500	9722	1439	550
chiral	4516	1884	0	314	105	12

TABLE 1. Statistics on integer eigenvalues and powers of U equalling the identity for regular and chiral maps on up to 1000 edges.

7. PERIODIC MAPS WITH $U^s = I$

It follows from Theorem 5.4 that any orientably-regular map which admits perfect state transfer or periodicity must have the property that some non-zero power of U is equal to the identity matrix. We searched all orientably-regular maps in the census of regular maps with at most 1000 edges [9] (up to duality and also up to mirror image for the chiral maps), and we found that many of them have the property that the matrix CC^T has all integer eigenvalues. For such maps, that are in particular type (k, d)-maps, $\widehat{C}\widehat{C}^T = \frac{1}{kd}CC^T$ has all rational eigenvalues. We also computed for each map, whether or not there exists some minimal $s \in \{1, 2, \dots, 1000\}$ such that $U^s = I$; only the values $s = 1, 2, 6, 12$ appeared in these computations. To give an idea of how common these properties are for regular and chiral maps, we summarize these computations in Table 1. In Section 8, we describe the computations in more detail. Because of these observations, we are motivated to study maps for which $U^s = I$ for some $s > 0$. In this section, we give necessary and sufficient conditions for $U^s = I$ when $s = 1, 2$ (Lemma 7.1, Lemma 7.2 and Corollary 7.3) and we give partial characterisations when $s > 2$ (Proposition 7.4 and Lemma 7.5). The section ends with a conjecture on a complete characterisation of the (minimal) s for which $U^s = I$ in orientably-regular maps (Conjecture 7.6). The results in this section support this conjecture.

A *quasi-tree* is an embedded graph with exactly one face. Dually, a *bouquet* is an embedded graph with exactly one vertex. A *quasi-tree bouquet* is a bouquet that is also a quasi-tree. Quasi-tree bouquets have been studied in various works, including [30, 11]. Lemma 7.1 gives another characterisation of quasi-tree bouquets, in terms of the unitary matrix of the vertex-face walk.

LEMMA 7.1. *The transition matrix satisfies $U = I$ if and only if the map is a quasi-tree bouquet.*

Proof. This follows from Theorem 5.1, part (ii) of Corollary 5.3, and duality. $\qquad\square$

Now, we turn our attention to the cases for which $U^s = I$ for some $s > 1$. The maps for which $U^2 = I$ are characterised in the following lemma. Recall our notation for $P = \widehat{M}\widehat{M}^T$ and $Q = \widehat{N}\widehat{N}^T$. Recall also that the vertex-face incidence matrix C is given by $C = N^T M$, where the (v, f)-entry of C is equal to the number of times the vertex v appears on the facial walk of the face f. Moreover, the normalized vertex-face incidence matrix $\widehat{C}$ is given by $\widehat{C} = \widehat{N}^T \widehat{M}$. Finally, $J_{A\times B}$ denotes the all-ones matrix indexed by sets A and B.

LEMMA 7.2. *The following are equivalent:*
  (i) $U^2 = I$;
  (ii) $PQ = |\mathcal{A}|^{-1} J_{\mathcal{A}\times\mathcal{A}}$;
  (iii) $C = |\mathcal{A}|^{-1} D J_{V\times F} \Delta$;
  (iv) $\widehat{C}\widehat{C}^T = |\mathcal{A}|^{-1} D^{\frac{1}{2}} J_{V\times V} D^{\frac{1}{2}}$;
  (v) *every vertex v is traversed $|\mathcal{A}|^{-1} d(v) d(f)$ times by the facial walk of every face f, where $d(v)$ is the degree of v and $d(f)$ is the degree of f.*

Proof. Note that (iii) and (v) are equivalent because of the combinatorial interpretation of C: the (v, f)-entry of C is equal to $|\mathcal{A}|^{-1} d(v) d(f)$. We will now show that (i), (ii), (iii) and (iv) are equivalent.

To show that (i) implies (ii), note that if $U^2 = I$, then U is symmetric. Since we can write

$$U = 4PQ - 2(P + Q) + I,$$

this implies that PQ must be symmetric. In particular, since P and Q are orthogonal projections, PQ is itself an orthogonal projection. Since P and Q are symmetric matrices themselves, we see that $PQ = (PQ)^T = QP$, so the image of PQ is $\mathrm{col}(N) \cap \mathrm{col}(M)$, which is equal to $\mathrm{span}\{\mathbf{1}_{\mathcal{A}}\}$ by Theorem 3.1(i). Thus PQ is the orthogonal projection onto $\mathrm{span}\{\mathbf{1}_{\mathcal{A}}\}$, that is $PQ = |\mathcal{A}|^{-1} J_{\mathcal{A}\times\mathcal{A}}$.

If (ii) holds, then, as we can write $N = QN$ and $M = PM$, we find that

$$C = N^T M = N^T QPM = |\mathcal{A}|^{-1} N^T J_{\mathcal{A}\times\mathcal{A}} M = |\mathcal{A}|^{-1} D J_{V\times F} \Delta,$$

so we see that (ii) implies (iii).

Now assume that (iii) holds. Then

$$\widehat{C} = D^{-\frac{1}{2}} C \Delta^{-\frac{1}{2}} = |\mathcal{A}|^{-1} D^{\frac{1}{2}} J_{V\times F} \Delta^{\frac{1}{2}},$$

so that

$$\widehat{C}\widehat{C}^T = |\mathcal{A}|^{-2} D^{\frac{1}{2}} J_{V\times F} \Delta J_{F\times V} D^{\frac{1}{2}} = |\mathcal{A}|^{-1} D^{\frac{1}{2}} J_{V\times V} D^{\frac{1}{2}},$$

proving (iv). Here, the last equality holds because every entry of $J_{V\times F} \Delta J_{F\times V}$ is equal to the sum of the face-degrees, which is $|\mathcal{A}|$.

Finally, assume that (iv) is true. Then $\widehat{C}\widehat{C}^T$ is a rank-one matrix that has 1 as an eigenvalue (with eigenvector $D^{\frac{1}{2}} \mathbf{1}_V$). In particular, $\widehat{C}\widehat{C}^T$ has no eigenvalues besides 0 and 1, so by Theorem 3.3, the eigenvalues of U are in $\{-1, 1\}$. This implies (i). $\qquad\square$

The cycle C_n embedded on the sphere is a type $(n, 2)$ map with n vertices and 2 faces. Every vertex is traversed once by the facial walk of either face and we have $U^2 = I$ by part (iv) of the above result. In general, we state a combinatorial characterisation of when $U^2 = I$ for a map of type (k, d) more simply in the following corollary.

COROLLARY 7.3. *If X is a type (k, d) map, then $U^2 = I$ if and only if every vertex is traversed by the facial walk of any face $k/|V| = d/|F|$ times.*

Proof. This follows directly from part (v) of Lemma 7.2. □

As is apparent from our computations in Section 8, the case $U^2 = I$ accounts for many examples of periodicity found amongst orientably-regular maps.

In the following proposition, we show that for $p > 2$ prime, type (k, d)-maps that have incidence multiplicity α can only have the property that $U^p = I$ under a very restricted set of circumstances.

PROPOSITION 7.4. *Let X be an orientable embedding of type (k, d) with incidence multiplicity α and let $p > 2$ be prime. If $U^p = I$, then exactly one of the following three cases holds:*

   (i) *$d = \alpha$ and $U = I$;*
   (ii) *$d = 2\alpha$, $|V| = |F| = p$ and α is even;*
   (iii) *$d = 3\alpha$, $p = 3$, $|V| = |F| = 9$ and α is divisible by 4.*

Proof. Throughout this proof, we will write $n = |V|$, $\ell = |E|$ and $s = |F|$. If $U^p = I$ for some odd prime p, then -1 is not an eigenvalue of U, hence we know by Corollary 3.2 that $n = s$. This also implies that $k = d$, as $nd = sk = |\mathcal{A}|$. Moreover, by Euler's formula,

$$n + s - \ell = 2 - 2g.$$

Since $n = s$, it must be that ℓ is even.

The eigenvalues of U that are unequal to 1 are primitive p-th roots of unity. Since U is a rational matrix, any eigenvalue must occur with the same multiplicity as each of its algebraic conjugates. Thus all eigenvalues of U not equal to 1 have the same multiplicity, say $m \geqslant 0$. The multiplicities of the eigenvalues add up to the dimension of the whole space, so

$$|\mathcal{A}| = m_1 + (p - 1)m = \ell + 2g + (p - 1)m,$$

where $m_1 = \ell + 2g$ is the dimension of the 1-eigenspace of U. Since $|\mathcal{A}| = 2\ell$, we find (using Euler's formula) that

$$(13) \qquad\qquad m(p - 1) = \ell - 2g = n + s - 2 = 2(n - 1).$$

Let $\theta_1, \ldots, \theta_d$ be the distinct eigenvalues of U, with corresponding multiplicities $m_1, \ldots, m_d$. We may assume that $\theta_1 = 1$, in which case $m_2 = \ldots = m_d = m$. The trace of U equals the sum of its eigenvalues, so we can write

$$\text{tr}(U) = m_1 + \sum_{i=2}^{d} m_i \theta_i = \ell + 2g + m \sum_{i=2}^{d} \theta_i = \ell + 2g - m$$

since the (non-trivial) primitive p-th roots of unity sum to -1. On the other hand, by Lemma 3.4, and the fact that $n = s$ and $k = d$, we can write

$$\text{tr}(U) = \frac{4\alpha n}{d} - 4n + |\mathcal{A}|$$

for the trace of U. From these two expressions for $\text{tr}(U)$, and Euler's formula, we obtain that

$$m = (\ell + 2g) - \left(\frac{4\alpha n}{d} - 4n + 2\ell \right) = 2n + 2 - \frac{4\alpha n}{d}.$$

We observe from (13) that m divides $n-1$, so m is at most $n-1$ and we may rearrange to obtain $3 \leqslant \frac{4\alpha n}{d} - n$, and thus $d < 4\alpha$. As d is a multiple of α, that leaves three possible values for d: $d = \alpha$, $d = 2\alpha$ or $d = 3\alpha$. If $d = \alpha$, then $k = \alpha$. Then every vertex is only incident to one face, and every face is only incident to one vertex. This implies that $n = s = 1$, in which case $U = I$ by Lemma 7.1. This is case (i). If $d > \alpha$,

then the map has more than one vertex and one face, so $U \neq I$ and hence $m > 0$. For $d = 2\alpha$, by (13) and our expression for m:

$$p - 1 = \frac{2n - 2}{2n + 2 - \frac{4\alpha n}{d}} = \frac{2n - 2}{2} = n - 1,$$

so $n = s = p$. As stated above, ℓ is even. In this case, we have $\ell = p\alpha$, so α must be even. This is case (ii).

Similarly, if $d = 3\alpha$, we find that

$$p - 1 = \frac{2n - 2}{2n + 2 - \frac{4n}{d}} = \frac{n - 1}{1 + \frac{n}{3}} = \frac{3n - 3}{n + 3} < 3.$$

Since $p > 2$, it must be that $p = 3$. Solving for n then gives $n = s = 9$. But now $2\ell = nd = 27\alpha$, so for ℓ to be even, we need that $\alpha = 0 \mod 4$. This is case (iii). $\square$

We note that this implies that maps of type (k, d) with an odd incidence multiplicity α (in particular circular embeddings), yield $U^p \neq I$ for all primes $p > 2$. Note that this includes all toroidal (m, n)-grids with $m, n \geqslant 2$, which we studied in Section 6.2.

In Proposition 7.4, the maps that satisfy case (i) are precisely all quasi-tree bouquets. For any $p > 2$, an example of case (ii) is the toroidal $(1, p)$-grid, which is discussed in Section 6.2. We do not know of any example of case (iii).

LEMMA 7.5. *Let X be a map for which the matrix $\widehat{C}\widehat{C}^T$ has rational eigenvalues. Assume that $U^\tau = I$ for some $\tau > 1$ and $U^s \neq I$ for all $s < \tau$, then $\tau \in \{2, 3, 4, 6, 12\}$.*

Proof. Let $\xi \neq 1$ be an eigenvalue of U. Then ξ is a primitive r-th root of unity for some r that divides τ. If also $\xi \neq -1$ (meaning that $r > 2$), then as ξ is an eigenvalue of U, it is a root of

$$p(t) = t^2 - (4\hat{\lambda} - 2)t + 1$$

for some eigenvalue $\hat{\lambda}$ of $\widehat{C}\widehat{C}^T$ by Theorem 3.3. By assumption this eigenvalue is rational, so $p(t)$ has rational coefficients. Then $p(t)$ must be the minimal polynomial of ξ over $\mathbb{Q}$. In particular, because ξ is a primitive root of unity, $p(t)$ is the r-th cyclotomic polynomial. It has degree 2, which implies that $r \in \{3, 4, 6\}$. Because τ is minimal, it is the least common multiple of some non-empty subset of $\{2, 3, 4, 6\}$, meaning that $\tau \in \{2, 3, 4, 6, 12\}$. $\square$

We note that the converse partly holds; if $U^\tau = I$ for some $\tau \in \{2, 3, 4, 6\}$ and $U^s \neq I$ for all $s < \tau$, then $\widehat{C}\widehat{C}^T$ has rational eigenvalues. The cyclotomic polynomial for the $2, 3, 4, 6$th roots of unity have degrees 1 or 2; any minimal polynomial for these roots over an extension field of the rationals will divide the cyclotomic polynomials. Since the cyclotomic polynomials are only degree 1 or 2, we can say exactly what the eigenvalues of $\widehat{C}\widehat{C}^T$ have to be. Let ξ be an eigenvalue of U which is a root of

$$p(t) = t^2 - (4\hat{\lambda} - 2)t + 1$$

for some eigenvalue $\hat{\lambda}$ of $\widehat{C}\widehat{C}^T$. If ξ is a third root of unity, then $p(t)$ must divide $t^2 + t + 1$ and thus $\hat{\lambda} = \frac{1}{4}$. Similarly, if ξ is a fourth root of unity, then $p(t)$ must divide $t^2 + 1$ and thus $\hat{\lambda} = \frac{1}{2}$. If ξ is a sixth root of unity, then $p(t)$ must divide $t^2 - t + 1$ and $\hat{\lambda} = \frac{3}{4}$. Thus if every eigenvalue of U is ± 1 or a 3rd, 4th or 6th root of unity, then $\widehat{C}\widehat{C}^T$ has only rational eigenvalues.

Based on our intuition gained from the computational findings and the results in this section, we proffer the following conjecture:

CONJECTURE 7.6. *Let X be an orientably-regular map, and let U be its transition matrix. If $s > 0$ is such that $U^s = I$ and $U^r \neq I$ for all $r < s$, then $s \in \{1, 2, 6, 12\}$.*

The partial results of this section support the conjecture, but some additional insights are necessary for its resolution.

8. COMPUTATIONS

In this section, we offer context and motivation for some of our results. Since vertex-face walks are not yet well-studied in the literature, we performed numerical experiments on a large set of orientably-regular maps to obtain intuition for their behaviour. For this, we used a census that includes all orientably-regular maps having at most 1000 edges, provided by Conder [8, 9, 7]. In this list, each map is given as a presentation of its automorphism group. We used SageMath [29] to compute the incidence matrices N and M for each map, and then NumPy [19] to compute the transition matrix U and analyse the vertex-face walk on that map. In doing so, we observed some noteworthy behaviour. For instance, for a large proportion of orientably-regular maps with up to 1000 edges, the transition matrix U satisfies the property that $U^2 = I$. This provides motivation for our characterisations of such maps in Lemma 7.2 and Corollary 7.3. For other instances of periodicity, we searched only up to a finite time of $t = 1000$; we found no time greater than $t = 12$ that occurs as a period within this range. See also Section 9, in which we discuss bounding the time of PST and periodicity as an open problem.

We observed that for the orientably-regular maps, periodicity occurred only with period $t \in \{1, 2, 6, 12\}$. By part (ii) of Corollary 5.3, periodic maps with period $t = 1$ have only one vertex. For such maps, $U = I$ only if $|F| = 1$, i.e. if the map is a quasi-tree bouquet (Lemma 7.1). For every even integer $\ell > 0$, there is exactly one orientably-regular map with ℓ edges that is a quasi-tree bouquet.

By Theorem 5.1, periodic maps with a period of $t = 2, 6$ or 12 satisfy $U^t = I$. It is interesting to note that for all of the maps that we found that satisfy $U^t = I$ with period $t = 6, 12$, the transition matrix U does not have any primitive 6th or 12th roots of unity as an eigenvalue. Moreover, all of the periodic maps are included in a large subset of maps for which the matrix CC^T has integer eigenvalues, which motivated Lemma 7.5. Tables 2 and 3 summarize our computations on reflexible and chiral maps, respectively. Each table shows the number of maps, of each class, that have integer eigenvalues, and in the last four columns, for each $t \in \{1, 2, 6, 12\}$, the number of maps for which t is the smallest time at which $U^t = I$. In these tables, the reflexible maps are considered up to duality, and the chiral maps up to both duality and mirror image.

The transition matrix of the dual of a map X is given by U^T, where U is the transition matrix of X; thus $U^t = I$ if and only if $(U^T)^t = I$. However the period of the periodicity may differ since the state spaces are different: if $t > 0$ is odd and there is periodicity with period $2t$ in X, it is possible that there is periodicity with period t in the dual. This did occur for some maps in the census, but only at $t = 1$ for maps with a single face and more than one vertex, hence $U^2 = I$ (Corollary 5.2). Because of this, the dual maps were omitted from the table, and we count the maps for which $U^t = I$, since it applies to both maps under duality.

We did not find any orientably-regular maps with perfect state transfer at time $t > 1$. There were, however, maps with perfect state transfer at time $t = 1$, and such maps satisfy both $U^2 = I$ and $|V| = 2$ by Theorem 5.4 and Proposition 5.5.

Results from this paper were used to simplify our computations; for example, Corollary 7.3 was used to quickly determine whether a map satisfies $U^2 = I$, and Corollary 4.3 was used to simplify computations regarding perfect state transfer and periodicity.

edges	maps	$\sigma(CC^T) \subset \mathbb{Z}$	periodicity			
			$U = I$	$U^2 = I$	$U^6 = I$	$U^{12} = I$
2-100	793	773	50	522	35	7
101-200	1378	1289	50	764	88	29
201-300	1689	1527	50	860	116	48
301-400	2175	1906	50	965	143	57
401-500	1865	1720	50	958	98	17
501-600	2935	2360	50	1095	233	116
601-700	2273	1966	50	1059	136	52
701-800	3879	3031	50	1195	266	132
801-900	2634	2319	50	1162	176	60
901-1000	2699	2355	50	1142	148	32

TABLE 2. This table shows the number of reflexible maps that admit periodicity, broken down into ranges of 100 edges. We checked for periodicity only up to a time of 1000, and found periodicity only with periods $1, 2, 6,$ or 12.

edges	maps	$\sigma(CC^T) \subset \mathbb{Z}$	periodicity			
			$U = I$	$U^2 = I$	$U^6 = I$	$U^{12} = I$
2-100	61	36	0	5	0	0
101-200	176	89	0	15	3	0
201-300	263	143	0	26	6	1
301-400	368	140	0	26	9	0
401-500	393	190	0	32	6	0
501-600	511	228	0	37	22	8
601-700	593	210	0	32	13	0
701-800	769	275	0	49	18	2
801-900	632	317	0	46	15	1
901-1000	750	256	0	46	13	0

TABLE 3. This table shows the number of chiral maps that admit periodicity, broken down into ranges of 100 edges. We checked for periodicity only up to a time of 1000, and found periodicity only with periods $1, 2, 6,$ or 12.

9. FURTHER DIRECTIONS AND OPEN PROBLEMS

The area of discrete-time quantum walks is a relatively new area and examples are needed in order to build intuition. In this work, we have used the census of regular maps [9] to explore many examples of two-reflection discrete-time quantum walks, more specifically vertex-face walks. We then proved results about these walks related to the combinatorial properties of the corresponding embeddings. Connections with the topological properties of the embeddings have yet to be fully explored. Godsil and Zhan [16] study another model of discrete-time quantum walk on a graph, where the first reflection serves as a 'coin flip' that depends on a rotation system assigned to the graph. Since this is equivalent to embedding the graph into an orientable surface, they perform computations that seem to show a correlation between properties of the so-called *average mixing matrix* and the genus of the corresponding embedding; the exact relation has yet to be formulated and proven. Similar computations can be done for the vertex-face walk, which could be an interesting direction for future

work. In this paper, we have focused mostly on periodicity and perfect state transfer in the vertex-face walk; we will now discuss future directions related to perfect state transfer.

It appears that perfect state transfer (abbreviated hereafter as PST for brevity) is a rare phenomenon. For every time $t > 0$ there exists at least one map which admits PST at time t, namely the toroidal $(1, 2t)$-grid as discussed in Section 6.2. For odd t there is also the toroidal $(2, t)$ grid with PST at time t. Besides toroidal grids, the only maps that we know to admit PST have the PST occurring at time 1 and are maps with only two vertices. We have also searched all orientable embeddings of cubic graphs on up to 12 vertices but PST did not occur for any of these maps. It would be interesting to see more examples of maps that admit PST. In particular, we do not know of any simple graphs admitting PST, other than the planar embedding of K_2. To aid in the quest for PST, the following open problem would be of interest:

OPEN PROBLEM 9.1. *Does there exist a constant upper bound on a time of PST, in a map admitting PST?*

In our computations involving the census of orientably-regular maps, we have searched for PST and periodicity only up to a time of 1000; we performed a limited number of computations, since we have limited computational resources and our main objective is not computational in nature.

The vertex-face walk is periodic if and only if some power of its transition matrix equals the identity. If we want to determine if some power of an arbitrary unitary matrix U, with rational entries, is the identity, note that it is not sufficient to check only the powers $U, U^2, \ldots, U^{|U|}$, where $|U|$ denotes the order of U. For example, the matrix $M = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ is a 2×2 with primitive 4th roots of unity as eigenvalues. However, for the vertex-face walk, if $U^s = I$, we can give a rough upper bound on s using the numbers of vertices and faces, which we show in Appendix A.

Another open problem would be to find a function $f(n, k, d)$ such that for a type (k, d)-map (or, indeed, a general map), if $U^s \neq I$ for all $s \leqslant f(n, k, d)$, then no power of U is the identity. For an orientably-regular map, this would imply that the map does not admit periodicity at any vertex at any time.

We found PST in the toroidal grids with $n = 1, 2$, but did not find it anywhere else. The symmetry of these maps implies that if there is uv-PST for some vertices u, v, then the vertex set must partition into pairs where there is PST between every pair. We make the following conjecture.

CONJECTURE 9.2. *Let $n, m \geqslant 3$ such that $(n, m) \neq (4, 4)$. Then the toroidal (n, m)-grid is not periodic at any time τ. Consequently, there is also no perfect state transfer at any time τ.*

Since perfect state transfer in vertex-face walks appears to be a rare phenomenon, we can turn our attention to the several other possible methods of state transfer. In the remainder of this section, we will discuss variations on the notion of PST for the vertex-face walk.

PST BETWEEN VERTICES OF DIFFERENT DEGREES. Recall that in Section 4, we originally defined PST between vertices u and v at time $\tau > 0$ as $U^\tau \widehat{N} \mathbf{e}_u = \mathbf{x}$ where $\mathbf{x} \in \mathbb{C}^{\mathcal{A}}$ is a unit length vector that satisfies $\widehat{N} \mathbf{e}_w \circ \mathbf{x} = 0$ for all $w \neq v$ (i.e. $\mathbf{x}$ is any superposition of the arcs incident to v). We then restricted the definition of PST to be between vertices u and v of equal degree, in which $\mathbf{x}$ would necessarily have to equal $\widehat{N} \mathbf{e}_v$ (Lemma 4.4). If we allow u and v to have different degrees however, $\mathbf{x}$ can be any superposition of the arcs that are incident to v. This raises the question: are
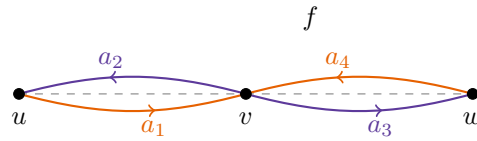
FIGURE 12. The vertex-face walk on P_3, with in blue the initial state $\widehat{N}\mathbf{e}_v$ and in red the state $R\widehat{N}\mathbf{e}_v$, at time 1.
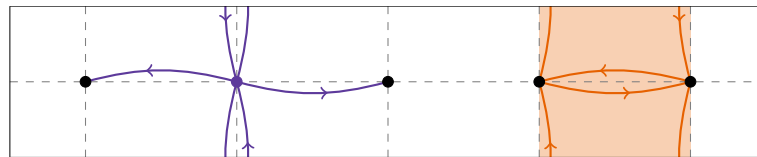

FIGURE 13. Vertex-face PST in the toroidal $(1,5)$-grid. The arcs incident to the purple vertex are sent to the arcs incident the orange face in 3 steps. The graph is drawn on the cut-open torus, where the opposite sides are identified; for visual simplicity, we have omitted the labels on the boundary of the torus.

there maps for which this more general type of uv-PST occurs between vertices of different degrees? As was discussed in Section 4, this can only happen if the degree of v is larger than the degree of u. We do not know of any examples of perfect state transfer between vertices of different degrees in a vertex-face walk.

"REVERSE" PST. Consider the unique genus 0 embedding of the path P_3 as depicted in Figure 12. Because P_3 is a tree, we have $U^2 = I$. Like for all trees other than K_2, there is also no PST at time 1. However, U sends the uniform superposition of the arcs incident to v to the reverse arcs:

$$U\widehat{N}\mathbf{e}_v = R\widehat{N}\mathbf{e}_v,$$

where R is the arc-reversal matrix. The same is true for the central vertex of any star graph $K_{1,n}$. Generally, we can say a map X admits *reverse uv-PST* at time τ if

$$U^\tau \widehat{N}\mathbf{e}_u = R\widehat{N}\mathbf{e}_v$$

for vertices u and v at some time $\tau > 0$. Besides the star graphs, this happens for any embedding of the graph on two vertices with a number of parallel edges between them, such as the digon from Figure 2. For all of these examples, the reverse-PST occurs at time $\tau = 1$. A natural problem to ask would be the following.

OPEN PROBLEM 9.3. *What are the classes of orientable maps that admit reverse uv-PST? Further, are there examples where it occurs for the first time at some time $\tau > 1$?*

VERTEX-FACE PST. Each step in the vertex-face walk on a map X can be thought of as taking one step in X and then one step in the dual X^*, each step corresponding to one of the two reflections that form the transition matrix U. It is hence natural to define a notion of state transfer between a vertex and a face; we say that a map admits *vertex-face perfect state transfer* if

$$U^\tau \widehat{N} e_u = \widehat{M} e_f$$

at some time $\tau > 0$ for some vertex u and face f.

For example, the toroidal $(1, 5)$-grid admits vertex-face perfect state transfer between the 'antipodal' vertex-face pairs, as shown in Figure 13. In this example, the map is periodic at time 5 and Lemma 5.3 tells us that $U^3 \widehat{N} e_u$ is in the column space of $\widehat{M}$; in fact, in this case, $U^3 \widehat{N} e_u$ is a column of $\widehat{M}$. Thus, in a sense, we can view the vertex-face PST as a strengthening of the condition in Lemma 5.3(i).

One can ask if it is easier to generate prolific examples of this form of PST. Other basic questions to investigate include the following:

- If vertex-face PST occurs at time τ, is there periodicity at time 2τ?
- If vertex-face PST occurs between vertex v and face f, can it also occur between v and $f' \neq f$ at some other time?
- What are some structural properties that v and f have to satisfy when vertex-face PST occurs between v and f?

For the third question, we are motivated by our example above, in which the vertex v and the face f are antipodal, in some sense.

APPENDIX A. BOUNDING THE MINIMAL TIME OF PERFECT STATE TRANSFER

If a map X has a partition of vertices into pairs, such that X admits perfect state transfer between every pair, then we can give a crude bound on the time of perfect state transfer, using some basic algebraic number theory. In the following lemma, φ denotes the Euler totient function.

LEMMA A.1. *If $U^s = I$ and $U^t \neq I$ for $0 < t < s$, then $2 \min\{n, f\} \geqslant \varphi(s')$ for any divisor s' of s such that there exists an eigenvalue of U which is a primitive s'th root of unity.*

Proof. Let $\psi(t) := \psi(\widehat{C}\widehat{C}^T, t)$ denote the minimal polynomial of $\widehat{C}\widehat{C}^T$. Since $\widehat{C}\widehat{C}^T$ has entries in $\mathbb{Q}$, the roots of $\psi(t)$ lie in some field extension of $\mathbb{Q}$; let $\mathbb{K}$ be the splitting field of ψ over $\mathbb{Q}$.

Let λ be an eigenvalue of U. By Theorem 3.3, the minimal polynomial of λ over $\mathbb{K}$ has degree at most 2. Let $\mathbb{L}$ be the splitting field of the minimal polynomial of λ over $\mathbb{K}$. Since $U^s = I$, we see that every eigenvalue of U must be an sth root of unity. Thus, for some s' dividing s, we have that λ is a primitive s'th root of unity and so $\lambda \in \mathbb{Q}(\zeta)$ where $\zeta = e^{\frac{2\pi i}{s'}}$. Since U is a rational matrix, its characteristic polynomial has rational coefficients and thus the algebraic conjugates of λ must occur as eigenvalues of U with equal multiplicity as λ and so we see that $\mathbb{Q}(\zeta) \subseteq \mathbb{L}$.

Now we consider the indices of these field extensions and we see that $[\mathbb{L} : \mathbb{K}] \leqslant 2$ and

$$[\mathbb{K} : \mathbb{Q}] \leqslant \deg(\psi(t)) \leqslant \min(n, f),$$

since $\widehat{C}\widehat{C}^T$ and $\widehat{C}^T\widehat{C}$ have the same minimal polynomial $p(t)$, up to a factor of t, and the degree is upper-bounded by size of the matrix. We also have that

$$[\mathbb{L} : \mathbb{Q}] = [\mathbb{L} : \mathbb{K}][\mathbb{K} : \mathbb{Q}] \geqslant [\mathbb{Q}(\zeta) : \mathbb{Q}] = \varphi(s')$$

where φ denotes the Euler totient function. $\qquad\square$

A well-known, elementary lower bound for the Euler totient function of a number n is $\varphi(n) \geqslant \sqrt{\frac{n}{2}}$. We obtain that $s' \leqslant 2(2\min\{n, f\})^2 = 8(\min\{n, f\})^2$. Let S be the set of integers s' such that U has an eigenvalue which is a primitive s'th root of unity. Since s is the smallest positive integer such that $U^s = I$, we see that s is the least common multiple of the elements of S. If s is prime, then $s \in S$ and we have that

$$s \leqslant 8(\min\{n, f\})^2.$$

Otherwise, the elements of S are each upper bounded by $8(\min\{n, f\})^2$ and thus

$$s \leqslant \prod_{s' \in S} s' \leqslant (8(\min\{n, f\})^2)!.$$

COROLLARY A.2. *If a map X has a partition of its vertices into pairs, such that X admits perfect state transfer between every pair, then the time τ where perfect state transfer first occurs is upper bounded as follows:*

$$\tau \leqslant \frac{1}{2}(8(\min\{n, f\})^2)!.$$

Proof. If X admits perfect state transfer at time τ between every pair of vertices, then X is periodic at time 2τ and, by Theorem 5.1, $U^{2\tau} = I$. By the discussion above, we see that $2\tau \leqslant (8(\min\{n, f\})^2)!$ and the result follows. $\square$

REFERENCES

[1] Andris Ambainis, Renato Portugal, and Nikolay Nahimov, *Spatial search on grids with minimum memory*, Quantum Inf. Comput. **15** (2015), no. 13-14, 1233–1247.

[2] Simon Apers, András Gilyén, and Stacey Jeffery, *A unified framework of quantum walk search*, 38th International Symposium on Theoretical Aspects of Computer Science, LIPIcs. Leibniz Int. Proc. Inform., vol. 187, Schloss Dagstuhl. Leibniz-Zent. Inform., Wadern, 2021.

[3] Leonardo Banchi, Gabriel Coutinho, Chris Godsil, and Simone Severini, *Pretty good state transfer in qubit chains—the Heisenberg Hamiltonian*, J. Math. Phys. **58** (2017), no. 3, article no. 032202 (9 pages).

[4] Ada Chan and Hanmeng Zhan, *Pretty good state transfer in discrete-time quantum walks*, J. Phys. A **56** (2023), no. 16, article no. 165305 (25 pages).

[5] Qiuting Chen, Chris Godsil, Mariia Sobchuk, and Harmony Zhan, *Hamiltonians of bipartite walks*, 2022, https://arxiv.org/abs/2207.01673.

[6] Andrew M. Childs, *On the relationship between continuous- and discrete-time quantum walk*, Comm. Math. Phys. **294** (2010), no. 2, 581–603.

[7] Marston Conder and Peter Dobcsányi, *Determination of all regular maps of small genus*, J. Combin. Theory Ser. B **81** (2001), no. 2, 224–242.

[8] Marston D. E. Conder, *Regular maps and hypermaps of Euler characteristic −1 to −200*, J. Combin. Theory Ser. B **99** (2009), no. 2, 455–459.

[9] ———, *Rotary maps (on orientable or non-orientable surfaces) with up to 1000 edges*, 2012, https://www.math.auckland.ac.nz/~conder/RotaryMapsWithUpTo1000Edges.txt.

[10] G. Coutinho, C. Godsil, K. Guo, and F. Vanhove, *Perfect state transfer on distance-regular graphs and association schemes*, Linear Algebra Appl. **478** (2015), 108–130.

[11] Mark N. Ellingham and Joanna A. Ellis-Monaghan, *A catalog of enumeration formulas for bouquet and dipole embeddings under symmetries*, Symmetry **14** (2022), no. 9, article no. 1793 (39 pages).

[12] Matthew Falk, *Quantum search on the spatial grid*, 2013, https://arxiv.org/abs/1303.4127.

[13] Chris Godsil and Krystal Guo, *Quantum walks on regular graphs and eigenvalues*, Electron. J. Combin. **18** (2011), no. 1, article no. 165 (9 pages).

[14] Chris Godsil, Krystal Guo, Mark Kempton, Gabor Lippner, and Florentin Münch, *State transfer in strongly regular graphs with an edge perturbation*, J. Combin. Theory Ser. A **172** (2020), article no. 105181 (27 pages).

[15] Chris Godsil, Stephen Kirkland, Simone Severini, and Jamie Smith, *Number-theoretic nature of communication in quantum spin systems*, Phys. Rev. Lett. **109** (2012), no. 5, article no. 050502.

[16] Chris Godsil and Hanmeng Zhan, *Discrete-time quantum walks and graph structures*, J. Combin. Theory Ser. A **167** (2019), 181–212.

[17] _____ , *Discrete quantum walks on graphs and digraphs*, London Mathematical Society Lecture Note Series, vol. 484, Cambridge University Press, Cambridge, 2023.

[18] Jonathan L. Gross and Thomas W. Tucker, *Topological graph theory*, Wiley-Interscience Series in Discrete Mathematics and Optimization, John Wiley & Sons, Inc., New York, 1987, A Wiley-Interscience Publication.

[19] Charles R. Harris, K. Jarrod Millman, Stéfan J. van der Walt, Ralf Gommers, Pauli Virtanen, David Cournapeau, Eric Wieser, Julian Taylor, Sebastian Berg, Nathaniel J. Smith, Robert Kern, Matti Picus, Stephan Hoyer, Marten H. van Kerkwijk, Matthew Brett, Allan Haldane, Jaime Fernández del Río, Mark Wiebe, Pearu Peterson, Pierre Gérard-Marchant, Kevin Sheppard, Tyler Reddy, Warren Weckesser, Hameer Abbasi, Christoph Gohlke, and Travis E. Oliphant, *Array programming with NumPy*, Nature **585** (2020), no. 7825, 357–362.

[20] Stacey Jeffery and Sebastian Zur, *Multidimensional quantum walks, with application to k-distinctness*, 2023, `https://arxiv.org/abs/2208.13492`.

[21] Neil B. Lovett, Sally Cooper, Matthew Everitt, Matthew Trevers, and Viv Kendon, *Universal quantum computation using the discrete-time quantum walk*, Phys. Rev. A (3) **81** (2010), no. 4, article no. 042330 (7 pages).

[22] Frédéric Magniez, Ashwin Nayak, Jérémie Roland, and Miklos Santha, *Search via quantum walk*, SIAM J. Comput. **40** (2011), no. 1, 142–164.

[23] Bojan Mohar and Carsten Thomassen, *Graphs on surfaces*, Johns Hopkins Studies in the Mathematical Sciences, Johns Hopkins University Press, Baltimore, MD, 2001.

[24] Apoorva Patel, K. S. Raghunathan, and Pranaw Rungta, *Quantum random walks do not need a coin toss*, Phys. Rev. A (3) **71** (2005), no. 3, article no. 032347 (6 pages).

[25] Renato Portugal, *Quantum walks and search algorithms*, second ed., Quantum Science and Technology, Springer, Cham, 2018.

[26] Theodore J. Rivlin, *The Chebyshev polynomials*, Pure and Applied Mathematics, Wiley-Interscience [John Wiley & Sons], New York-London-Sydney, 1974.

[27] Miklos Santha, *Quantum walk based search algorithms*, Theory and applications of models of computation, Lecture Notes in Comput. Sci., vol. 4978, Springer, Berlin, 2008, pp. 31–46.

[28] Mario Szegedy, *Quantum speed-up of Markov chain based algorithms*, 45th Annual IEEE Symposium on Foundations of Computer Science (Los Alamitos CA), IEEE, 2004, pp. 32–41.

[29] The Sage Developers, *Sagemath, the Sage Mathematics Software System (Version 9.0)*, 2020, `https://www.sagemath.org`.

[30] Qi Yan and Xian'an Jin, *A-trails of embedded graphs and twisted duals*, Ars Math. Contemp. **22** (2022), no. 2, article no. 6 (16 pages).

[31] Hanmeng Zhan, *Quantum walks on embeddings*, J. Algebraic Combin. **53** (2021), no. 4, 1187–1213.

KRYSTAL GUO, Korteweg-de Vries Institute for Mathematics, University of Amsterdam, Amsterdam, The Netherlands, and QuSoft (Research center for Quantum software & technology), Amsterdam, The Netherlands
E-mail : `k.guo@uva.nl`

VINCENT SCHMEITS, Korteweg-de Vries Institute for Mathematics, University of Amsterdam, Amsterdam, The Netherlands
E-mail : `v.f.schmeits@uva.nl`