Localization of two dimensional quantum walks defined by generalized Grover coins

Amrita Mandal∗, Rohit Sarma Sarkar †, Bibhas Adhikari‡

Abstract. Localization phenomena of quantum walks makes the propagation dynamics of a walker strikingly different from that corresponding to classical random walks. In this paper, we study the localization phenomena of four-state discrete-time quantum walks on two-dimensional lattices with coin operators as one-parameter orthogonal matrices that are also permutative, a combinatorial structure of the Grover matrix. We show that the proposed walks localize at its initial position for canonical initial coin states when the coin belongs to classes which contain the Grover matrix that we consider in this paper, however, the localization phenomena depends on the coin parameter when the class of parametric coins does not contain the Grover matrix.

Keywords. Quantum walk, Grover matrix, Localization

1 Introduction

In this paper, we study the localization phenomena of discrete-time four-state quantum walks on two dimensional lattices with parametric coin operators as orthogonal permutative matrices (OPMs) of order 4, which we call generalized Grover coins. An orthogonal permutative matrix is an orthogonal matrix whose any row is a permutation of any other row, a property of the well-known Grover matrix $G = \frac{1}{2} \left( I_4 \right)$ where $I_4$ denotes the all-one (column) vector of dimension 4 and $I_4$ is the identity matrix of order 4. We call the proposed walks as generalized Grover walks. The set of all OPMs of order 4 is denoted as $\mathcal{OP}_4$.

A discrete-time quantum walk (DTQW) is governed by the repeated application of a unitary operator $U = S_f (C \otimes I)$ to the initial state of the walker, where $S_f$ is the shift operator, $C$ is called the coin operator, and $\otimes$ denotes the Kronecker (also known as tensor) product of matrices. Thus the evolution operator $U$ of a proposed walk acts on the Hilbert space, which is the tensor product of the position space spanned by the quantum states localized at the vertices of the lattice and the coin space whose dimension 4 gives the internal degree of freedom of the quantum coin. A coined walk is called the Grover walk if coin operator is the Grover matrix. In this paper, we particularly focus on the proposed walks when the coin operator $C \in X_\theta \cup Y_\theta \cup Z_\theta \subset \mathcal{OP}_4$, where

$$X_\theta = \left\{ \begin{bmatrix} \frac{1}{2} \sin \theta & -\frac{1}{2} \sin \theta & \frac{1}{2} (1 + \cos \theta) & \frac{1}{2} (1 - \cos \theta) \\ -\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} (1 - \cos \theta) & \frac{1}{2} (1 + \cos \theta) \\ \frac{1}{2} (1 - \cos \theta) & \frac{1}{2} (1 + \cos \theta) & \frac{1}{2} \sin \theta & -\frac{1}{2} \sin \theta \\ \frac{1}{2} (1 + \cos \theta) & -\frac{1}{2} \sin \theta & -\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta \end{bmatrix} : \theta \in [-\pi, \pi] \right\},$$

$$Y_\theta = \left\{ \begin{bmatrix} \frac{1}{2} \sin \theta & \frac{1}{2} (1 + \cos \theta) & -\frac{1}{2} \sin \theta & \frac{1}{2} (1 - \cos \theta) \\ \frac{1}{2} (1 - \cos \theta) & \frac{1}{2} \sin \theta & \frac{1}{2} (1 + \cos \theta) & -\frac{1}{2} \sin \theta \\ -\frac{1}{2} \sin \theta & \frac{1}{2} (1 - \cos \theta) & \frac{1}{2} \sin \theta & \frac{1}{2} (1 + \cos \theta) \\ \frac{1}{2} (1 + \cos \theta) & -\frac{1}{2} \sin \theta & -\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta \end{bmatrix} : \theta \in [-\pi, \pi] \right\}. $$

∗Department of Mathematics, IIT Kharagpur, Email: mandalamrita55@gmail.com
†Department of Mathematics, IIT Kharagpur, Email: rohit15sarkar@yahoo.com
‡Corresponding author, Department of Mathematics, IIT Kharagpur, Email: bibhas@maths.iitkgp.ac.in
and the conditional shift operator moves the walker to an adjacent position based on its coin state (see Section 2). We emphasize that the parametric matrices in $X_\theta, Y_\theta$, and $Z_\theta$ can be treated as continuous deformations of the Grover matrix of order 4 since $C = G$ for $\theta = -\pi/2$ [13].

In a few occasions in the literature the Grover walk is generalized by considering coin operators as parametric unitary matrices, which include the Grover matrix as a special case for some particular values of the parameters [21, 11, 12]. In [17], the parametric coin operators for three-state quantum walks are proposed by deforming the eigenvalues and the eigenvectors of the Grover matrix. Recently we have proposed to generalize three-state Grover walk on one-dimensional lattice and on cycle graphs by considering orthogonal permutative matrices of order 3 as parametric coins in [15, 14]. The only existing parametric coin operators of order 4 in the literature is first reported in [3], and limit distribution and localization of the quantum walks on two-dimensional lattices defined by these parametric coins are studied in [21]. However, our proposal of parametric OPMs as coin operators is significantly different from existing parametric coin operators in literature [3]. The parametric coins that we consider in this paper preserve the combinatorial structure of the Grover matrix i.e. the permutative structure of the Grover coin and the proposed coins also can be expressed as linear combinations of permutation matrices (see [13]) which have suitable quantum circuit representation [1].

It is pertinent to investigate whether the characteristics of the Grover walk extend to generalized Grover walks. The localization phenomena of the walker of a quantum walk at a given position is concerned with finding the walker at that position with a nonzero probability even if the number of walking time-steps tends to infinity [8, 20, 10]. In this paper, we analyze whether the localization property of the Grover walk [19] extends to the proposed generalized Grover walks. We also investigate how does the probability of finding the walker at a given position depend on the values of the coin parameter for the proposed quantum walks. A brief discussion on localization property is given in Section 2.

We show that the proposed walks on infinite lattice exhibit the localization phenomena at the initial position for canonical initial coin states when the coin operator $C \in X_\theta \cup Y_\theta \cup Z_\theta$. Thus we show that the walker can be found at the initial position, which is considered as the vertex $(0,0)$ of the infinite lattice, with a nonzero total time-averaged probability (defined in Section 2). This phenomena is also called trapping of the walker [22, 5, 6]. Next we demonstrate how does this probability value varies with the value of the coin parameter $\theta \in [-\pi, \pi]$ for a fixed choice of the initial state. We observe that the maximum and minimum probability values are attained at $\theta = 0$ or $\theta = \pm \pi$ when $C \in Y_\theta \cup Z_\theta$, i.e. coins are permutation matrices and if $C \in X_\theta$, the maximum and minimum values of the probability are attained at $\theta = \pm \pi/2$ or $0$ or $\pm \pi$, i.e. coins are $G, P_{12|34} G$ or permutation matrices. Here $P_\sigma$ denotes the permutation matrix associated with the permutation $\sigma \in S_4$, the symmetric group of order 4. Indeed, the $ij$ entry of $P_\sigma$ is 1 if $\sigma(i) = j$, otherwise it is 0. Later we derive all initial coin states for which the underlying walks with the coins from $Y_\theta \cup Z_\theta$ have a zero time-averaged probability at the initial position i.e. the origin of the infinite lattice, and hence the walks do not exhibit localization for those initial coin states in contrast to our proof that a walk localizes for any initial coin state when the coin operator $C$ is chosen from $X_\theta$ and $C \neq G$. We also observe that even though the coins in $Y_\theta, Z_\theta$ are permutation scaling of coins in $X_\theta$ for any fixed value of $\theta$, to be precise, $Y_\theta = \{P_{23} A_\theta P_{23} : A_\theta \in X_\theta\}$ and $Z_\theta = \{P_{13} A_\theta P_{13} : A_\theta \in X_\theta\}$, the eigenpairs of the corresponding evolution operators are significantly different. Consequently, the probability of finding the walker varies with the choice of the coin from $X_\theta, Y_\theta, Z_\theta$ for a fixed value of $\theta$.

Finally, we show that localization property of the Grover walk corresponding to the canon-
ical initial coin states is not invariant under the permutative property of the coin by finding
a set of parametric coin matrices $W_\theta \subset \mathcal{O}_4$ given by

$$W_\theta = \left\{ \begin{array}{c|cccc}
\frac{1}{2}(1 + \cos \theta) & \frac{1}{2}(1 - \cos \theta) & \frac{1}{2} \sin \theta & -\frac{1}{2} \sin \theta \\
\frac{1}{2}(1 - \cos \theta) & \frac{1}{2}(1 + \cos \theta) & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta \\
\frac{1}{2} \sin \theta & -\frac{1}{2} \sin \theta & \frac{1}{2}(1 - \cos \theta) & \frac{1}{2}(1 + \cos \theta) \\
-\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2}(1 + \cos \theta) & \frac{1}{2}(1 - \cos \theta) \\
\end{array} \right\} : -\pi \leq \theta \leq \pi \right\} \tag{4}$$

for which quantum walks with canonical initial coin states do not exhibit localization for some
coins belonging to $W_\theta$. Note that $G \notin W_\theta$ for any $\theta \in [-\pi, \pi]$ and hence the matrices in $W_\theta$
need not be considered as continuous deformation of the Grover coin.

The organization of the remainder of the paper is as follows. In Section 2 we briefly discuss
the different notions of the localization property as considered in literature. Then we justify
the choice for the definition of localization which we consider in this paper. In Section 3
we study the localization property of the proposed quantum walks when the coin operator
belongs to $X_\theta, Y_\theta, Z_\theta$ and $W_\theta$. Then we conclude the paper.

2 Preliminaries

In this section, we discuss the mathematical machinery for analyzing the phenomena of
localization of the proposed walks. We first present a brief review of four-state DTQWs on
two-dimensional lattices following [3]. Then, we elaborate the notion of localization property
of DTQWs developed in several other articles in the literature.

Let

$$Z_N = \{(x, y) \in \mathbb{Z}^2 : -(N-1)/2 \leq x \leq (N-1)/2, -(N-1)/2 \leq y \leq (N-1)/2\}, \tag{5}$$

denote the square lattice with $N^2$ vertices, where $N$ is odd. Let $\mathcal{H}_p$ and $\mathcal{H}_c$ denote the $N^2$-
dimensional position space and four-dimensional coin space respectively. Then the proposed
walk is defined by the states of the walker as $|\psi(t)\rangle = U|\psi(t-1)\rangle = U^t |\psi(0)\rangle$, $t \geq 1$ where the
evolution operator is given by $U = S_f(C \otimes I)$ with initial state $|\psi(0)\rangle$, $S_f = \sum_{(x,y) \in Z_N} S_{x,y}$
where

$$S_{x,y} = |R\rangle \langle R| \otimes |x - 1(\text{mod}N), y\rangle \langle x, y| + |L\rangle \langle L| \otimes |x + 1(\text{mod}N), y\rangle \langle x, y|$$

$$+ |U\rangle \langle U| \otimes |x, y - 1(\text{mod}N)\rangle \langle x, y| + |D\rangle \langle D| \otimes |x, y + 1(\text{mod}N)\rangle \langle x, y|,$$

represents the conditional shift operator and $C$ denotes the coin operator. Besides, $|R\rangle = |1\rangle, |L\rangle = |2\rangle, |U\rangle = |3\rangle, |D\rangle = |4\rangle$ denote the chirality of the walker: right, left, up and
down respectively, where $\{1, 2, 3, 4\}$ denotes the canonical orthonormal ordered basis
of the Hilbert space $\mathcal{H}_c$. Then corresponding to the orthonormal basis $\{|S, x, y\rangle : S \in \{R, L, U, D\}, (x, y) \in Z_N\}$ of the total state space, the state of the walker at time $t$ can be
written as

$$|\psi(t)\rangle = \sum_{S \in \{R, L, U, D\}} \sum_{(x,y) \in Z_N} \alpha_{|S, x, y\rangle} |S, x, y\rangle.$$

Then it may be noted that the basis element $|S, x, y\rangle = |S\rangle \otimes |(x, y)\rangle$ can be identified with
a canonical basis element $|j\rangle$, $1 \leq j \leq 4N^2$ of $4N^2$-dimensional Hilbert space $\mathbb{C}^{4N^2}$ by
$j = 4Ny + 4x + l(S) + 2N^2 - 2$ and $l(S) = 1, 2, 3, 4$ for $S = R, L, U, D$ respectively, see [3].

Thus the probability of finding the walker at a vertex $(x, y)$ at time $t$ is given by

$$P_t((x, y); \psi(0)) = \| |\psi(x, y\rangle(t)\|_2^2 = \sum_{S \in \{R, L, U, D\}} |\alpha_{|S, x, y\rangle}|^2$$

where the initial state $|\psi(0)\rangle$ is known and

$$|\psi_{x, y\rangle}(t) = \sum_{S \in \{R, L, U, D\}} \alpha_{|S, x, y\rangle} |S\rangle$$

(7)
corresponds to the vector \([\alpha_{R,x,y;t}, \alpha_{L,x,y;t}, \alpha_{U,x,y;t}, \alpha_{D,x,y;t}]^T\) of \(\mathbb{C}^4\). Then following [3], we define localization of the walk at a vertex \((x, y) \in \mathbb{Z}_N\) with the help of time-averaged probability
\[
\mathcal{P}_t((x, y); \psi(0)) = \frac{1}{T} \sum_{i=0}^{T-1} P_i((x, y); \psi(0)), T \geq 1
\] (8)
as follows.

**Definition 2.1.** The proposed walk localizes at a vertex \((x, y) \in \mathbb{Z}_N\) for some initial state \(|\psi(0)\rangle\) if the total time-averaged probability
\[
\mathcal{P}_N((x, y); \psi(0)) = \lim_{T \to \infty} \mathcal{P}_t((x, y); \psi(0)) > 0.
\]

For infinite lattice, the walk localizes at a vertex \((x, y)\) if total time-averaged probability
\[
\mathcal{P}_\infty((x, y); \psi(0)) = \lim_{N \to \infty} \mathcal{P}_N((x, y); \psi(0)) > 0.
\]

The operational meaning of total time-averaged probability is that it captures the proportion of time which the walker “spends” in any given node \((x, y)\) of the lattice for any initial state \(|\psi(0)\rangle\). We emphasize that localization is defined in the literature in several other ways [2, 16, 18]. For instance, localization is defined in [18] if \(\lim \sup_{t \to \infty} P_t((x, y); \psi(0)) > 0\) for quantum walks with periodic evolution operator on infinite lattice and it can be determined using the eigenvector projection operators. However, computing eigenfunctions of operators defined on infinite dimensional spaces is challenging. On the other hand, it is easy to verify that if the walk localizes according to Definition 2.1 then it also localizes according to the definition of localization used in [18].

Further, note that
\[
\mathcal{P}_N((x, y); \psi_S(0)) = \sum_{S' \in \{R, L, U, D\}} \mathcal{P}_N(S', (x, y); \psi_S(0)),
\]
where
\[
\mathcal{P}_N(S', (x, y); \psi_S(0)) = \lim_{T \to \infty} \frac{1}{T} \sum_{i=0}^{T-1} |\alpha_{S', x,y,i}|^2
\] (9)
denotes the time-averaged probability for the walker to be found at \((x, y)\) with a given coin state \(|S'\rangle\) and \(|\psi_S(0)\rangle\) denotes the initial state of the walker with \(|S\rangle\) as the initial coin state. Then the walk is localized if \(\mathcal{P}_N(S', (x, y); \psi_S(0)) > 0\) for some \(S'\). Obviously, equation (9) is valid for infinite lattice by considering \(N \to \infty\).

The Grover walk, when the coin operator is the Grover matrix, is well studied in literature [3, 7]. It is shown that localization of Grover walk on two-dimensional infinite lattice depends on initial state of the walk and it is also speculated that the asymptotic behavior of the walk depends on the eigenvalues of the evolution operator. Then, based on the degeneracy of eigenvalues of the evolution operator, a necessary and sufficient condition is obtained in [18] for quantum walks on infinite lattices corresponding to periodic evolution operator that does not localize at any vertex.

It is found that the eigenvalues of the evolution matrix \(U\) for the Grover walk can be derived from the eigenvalues of another matrix \(U_{n,m} = D_{n,m}G\) using Fourier transform, where \(D_{n,m}\) is a unitary diagonal matrix and \(G\) is the Grover matrix [3]. The same holds true when the Grover matrix is replaced by generalized Grover coins as described in the following proposition. The proof is similar to the case when the coin operator is of order 3 as considered in [15], hence we omit the proof.

**Proposition 2.2.** The two dimensional quantum walk operator \(U = S_f(C \otimes I)\) has eigenvalues \(\lambda_{n,m,j}\) with a corresponding eigenvector \(|\eta_{n,m,j}\rangle = |v_{n,m,j}\rangle \otimes |\phi_n, \phi_m'\rangle\) where \(\lambda_{n,m,j}\) is an eigenvalue of \(U_{n,m} = D_{n,m}C\) corresponding to an eigenvector \(|v_{n,m,j}\rangle\), \(|\phi_n\rangle\) = \(\sum_{x=-\frac{N}{2}}^{\frac{N}{2}} e^{-ikx} |x\rangle\), and
|φ′⟩ = ∑_{y=−N−1}^{N−1} e^{-ik'y}|y⟩; k = \frac{2\pi n}{N}, k' = \frac{2\pi m}{N}, n, m \in \{0, 1, \ldots, N − 1\}, and D_{n,m} = \text{diag}(\omega^n, \omega^{-n}, \omega^{-m}, \omega^m) where \omega = e^{\frac{2\pi i}{N}} for i = \sqrt{-1}.

Then the following corollary describes each entry of eigenvectors of U from the eigenvectors of U_{n,m}.

**Corollary 2.3.** Let \((\lambda_{n,m,k}, |\eta_{n,m,k}\rangle), k \in \{1, 2, 3, 4\}, n, m \in \{0, 1, \ldots, N − 1\} denote eigenpairs of U. If |\eta_{n,m,k}\rangle = [\eta_{r,n,m,k}], r = 1, \ldots, 4N^2 then

\[
\eta_{r,n,m,k} = \frac{v_{s,n,m,k}\omega^{-(nx+my)}}{N\|v_{n,m,k}\|_2},
\]

where \((x, y) \in Z_N\) and \(s \in \{1, 2, 3, 4\}\) satisfy \(r = 4Ny+4x+s+2N^2-2\) and \(v_{n,m,k} = [v_{s,n,m,k}]\) is an eigenvector of \(U_{n,m}\) associated with the eigenvalue \(\lambda_{n,m,k}\).

It is obvious to check that the eigenvectors of U as described in Proposition 2.2 are orthonormal.

### 3 Localization of two dimensional four state quantum walks with generalized Grover coins

In this section, we investigate localization phenomena of the proposed walks. First, we consider the walks defined by coins from \(Y_\theta, X_\theta, Z_\theta\) and then for coins from \(W_\theta\), when \(\theta \in [-\pi, \pi]\). We establish that the walks with coins from \(Y_\theta, X_\theta, Z_\theta\) exhibit the localization property at the initial position \((0, 0) \in \mathbb{Z} \times \mathbb{Z}\) for the given canonical initial coin states after providing a computable formula of the total time-averaged probability for each \(\theta\). Obviously, total time-averaged probability depends on the eigenpairs of the evolution operator. For finite lattice, the time-averaged probability also depends on the size of the lattice, and hence we focus on the infinite lattice and the total time-averaged probability is computed by approximating it using an integral formula. Indeed, the formula depends on the eigenvectors corresponding to constant eigenvalues and the initial state of the evolution operator (see Remark 3.14). Moreover, we characterize those initial states for which the time-averaged probability has zero or nonzero value at the position \((0, 0)\). Finally, the influence of the coin operator is observed for a fixed initial state by plotting the total time-averaged probability for several values of the coin parameter, which is one of the prime objectives of the paper.

#### 3.1 With coins from \(Y_\theta\)

Consider the walks when the coin operator \(C \in Y_\theta, \theta \in [-\pi, \pi]\). Note that if \(U = S_f(C \otimes I)\) denotes the evolution operator then

\[
U_{n,m} = D_{n,m}C = \begin{bmatrix}
\frac{1}{2} \sin \theta \omega^n & \frac{1}{2} \cos \theta \omega^{-n} & -\frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} \cos \theta \omega^n \\
\frac{1}{2} \cos \theta \omega^n & \frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} \cos \theta \omega^n & \frac{1}{2} \sin \theta \omega^{-n} \\
\frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} \cos \theta \omega^m & \frac{1}{2} \sin \theta \omega^m & \frac{1}{2} \cos \theta \omega^{-m} \\
\frac{1}{2} \cos \theta \omega^m & \frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} \cos \theta \omega^{-m} & \frac{1}{2} \sin \theta \omega^m
\end{bmatrix}.
\]  

(10)

First we derive the eigenvalues of \(U_{n,m}, n, m \in \{0, \ldots, 4N - 1\}\) as follows.

**Lemma 3.1.** Consider \(U_{n,m}\) from equation (10), where \(\theta \neq 0, \pm \pi\). Then a complete set of orthogonal eigenpairs \((\lambda_{n,m,k}, |v_{n,m,k}\rangle), k = 1, \ldots, 4\) of \(U_{n,m}\) are

\[
\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = \sin \theta (\cos \zeta_n + \cos \zeta_m) \pm i \sqrt{4 - \sin^2 \theta (\cos \zeta_n + \cos \zeta_m)^2},
\]

\[
\lambda_{n,m,4} = \frac{\sin \theta (\cos \zeta_n + \cos \zeta_m) \pm i \sqrt{4 - \sin^2 \theta (\cos \zeta_n + \cos \zeta_m)^2}}{2},
\]
\[|v_{n,0,k}\rangle = \begin{cases} 
(1 + \cos \theta + \sin \theta)\omega^{-n} - (1 + \cos \theta + \sin \theta) , & \text{if } k = 1 \\
(1 + \cos \theta)\omega^{-n} + \sin \theta , & \text{if } k = 2 \\
(1 + \cos \theta - \sin \theta)\omega^{-n} - \sin \theta , & \text{if } k = 3, 4,
\end{cases} \]

if \( n > 0 \), and

\[|v_{n,m,k}\rangle = \begin{cases} 
(1 + \cos \theta)\lambda_{n,m,k}\omega^{-m} - \sin \theta , & \text{if } k = 1 \\
(1 + \cos \theta - \sin \theta)\lambda_{n,m,k}\omega^{-m} - \sin \theta , & \text{if } k = 2 \\
(1 + \cos \theta)\lambda_{n,m,k}\omega^{-m} - \sin \theta , & \text{if } k = 3, 4,
\end{cases} \]

if \( n,m > 0 \) and \( k \in \{1, 2, 3, 4\} \), where \( \zeta_q = 2\pi q/N, q \in \{m,n\} \).

**Proof:** Note that \( \omega^q = e^{i\zeta_q} \). We also note that the characteristic polynomial of \( U_{n,m} \) is given by

\[ \chi_{U_{n,m}}(\lambda) = \lambda^4 - \sin \theta(\cos \zeta_m + \cos \zeta_n)\lambda^3 + \sin \theta(\cos \zeta_m + \cos \zeta_n)\lambda - 1. \]

By calculating the roots, we get the eigenvalues and the corresponding eigenvectors can be obtained by solving the system of equations \( (U_{n,m} - \lambda_{n,m,k}I_4)X = 0 \) for \( X \). Since \( U_{n,m} \) is a unitary matrix, eigenvectors of \( U_{n,m} \) corresponding to different eigenvalues are orthogonal. \( \square \)

**Lemma 3.2.** Consider \( U_{n,m} \) from equation (10), where \( \theta = 0, \pm \pi \). Then the set of orthogonal eigenpairs \((\lambda_{n,m,k}, |v_{n,m,k}\rangle)\), \( k = 1, \ldots, 4 \) of \( U_{n,m} \) are as follows. For \( \theta = 0 \),

\[ \lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = -i, \lambda_{n,m,4} = i, \]

\[ |v_{n,m,k}\rangle = [\lambda_{n,m,k}\omega^{-m}, \lambda_{n,m,k}\omega^{n-m}, \lambda_{n,m,k}\omega^{-m}, 1]^T, \]

and for \( \theta = \pm \pi \),

\[ \lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = -i, \lambda_{n,m,4} = i, \]

\[ |v_{n,m,k}\rangle = [\lambda_{n,m,k}\omega^{-n}, \lambda_{n,m,k}\omega^{m-n}, \lambda_{n,m,k}\omega^{-m}, 1]^T, \]

where \( \zeta_q = 2\pi q/N \) and \( \omega^q = e^{i\zeta_q}, q \in \{m,n\} \).

**Proof:** The proof is computational and easy to verify. \( \square \)

Then \( |\eta_{n,m,k}\rangle, 1 \leq k \leq 4, 0 \leq m,n \leq N - 1 \) form a set of orthonormal eigenvectors corresponding to the eigenvalues \( \lambda_{n,m,k} \) of \( U \), and hence

\[ U = \sum_{n,m,k} \lambda_{n,m,k} |\eta_{n,m,k}\rangle \langle \eta_{n,m,k}|. \]
Consequently, 
\[
|\psi(t)\rangle = U^t |\psi(0)\rangle = \sum_{n,m,k} \lambda_{n,m,k}^t |\eta_{n,m,k}\rangle \langle \eta_{n,m,k}| |\psi(0)\rangle 
\]
\[
= \sum_{j=1}^{4N^2} \sum_{n,m,k} \lambda_{n,m,k}^t \eta_{n,m,k} \psi_j(0) |\eta_{n,m,k}\rangle 
\]
\[
= \sum_{j=1}^{4N^2} \sum_{n,m,k} \sum_{S \in \{R,L,U,D\}} \sum_{(x,y) \in \mathbb{Z}_N} \lambda_{n,m,k}^t \eta_{j,n,m,k} \psi_j(0) \eta_{r,m,n,k} |S,x,y\rangle , 
\]
where \( r = 4Ny + 4x + l(S) + 2N^2 - 2 \). Then since the eigenvectors of the proposed evolution operator \( U \) can be obtained by the eigenvectors of \( U_{n,m} \) derived in Lemma 3.1, the wave function of the proposed DTWQ can be obtained by employing Corollary 2.3. Indeed,
\[
|\psi(t)\rangle = \sum_{S \in \{R,L,U,D\}} \sum_{(x,y) \in \mathbb{Z}_N} \alpha_{|S,x,y;t|} |S,x,y\rangle 
\]
where
\[
\alpha_{|S,x,y;t|} = \sum_{j=1}^{4N^2} \sum_{n,m,k} \lambda_{n,m,k}^t \eta_{j,n,m,k} \psi_j(0) \eta_{r,m,n,k} 
\]
(11)
where \( j = 4Ny' + 4x' + l(S') + 2N^2 - 2, \) and \( \psi_j(0) = \alpha_{|S',x',y';0|}, \ (x',y') \in \mathbb{Z}_N, S' \in \{R,L,U,D\} \). Then from equations (7) and (11) we have
\[
|\psi_{(x,y)}(t)\rangle = \frac{1}{N^2} \sum_{n,m,k} \lambda_{n,m,k}^t \frac{|v_{n,m,k}\rangle \langle v_{n,m,k}|}{\langle v_{n,m,k}|v_{n,m,k}\rangle} |\psi(0)\rangle \omega^{-(nx+my)}, 
\]
(12)
and \( P_t((x,y); \psi(0)) = \| |\psi(t)\rangle \|^2 \) follows from equation (6), which can be computed numerically. An explicit analytical expression of it in terms of the coin parameter \( \theta \) is hard to obtain due to the cumbersome expressions of eigenvectors \( |v_{n,m,k}\rangle \) of \( U_{n,m} \) given by Lemma 3.1.

We now consider calculating the total time-averaged probability for finding the walker at the initial position when the lattice is infinite following [3, 4]. We introduce some notations that enable us to derive a compact expression of \( P_t((x,y); \psi(0)) \) utilizing the fact that eigenvalues of \( U \) are repeated for different pairs of \((n,m)\). We refer to different coefficients \( \alpha_{|S,x,y;t|} \) given in equation (11) as follows:
\[
C_{r,j,0,0,k} = \frac{\langle \psi_{(S),0,0,k}|\psi_{(S'),0,0,k}\rangle}{\langle v_{0,0,0}|v_{0,0,0}\rangle}, \quad C_{r,j,n,m,k} = \sum_{(n',m') \in \Omega(n,m)} \frac{\langle \psi_{(S),n',m',k}|\psi_{(S'),n',m',k}\rangle}{\langle v_{n',m',k}|v_{n',m',k}\rangle} 
\]
(13)
where the second expression is defined for \( n > 0 \) and \( m > 0 \), and \( \Omega(n,m) = \{(n',m') : \Lambda(U_{n,m}) = \Lambda(U_{n',m'})\} \). Indeed, \( \Omega(n,m) = \{(n,0),(0,n),(N-n,0),(0,N-n); 0 \leq m < n \} \) if \( m = 0 \); \( \Omega(n,m) = \{(n,n),(n,N-n),(N-n,n),(N-n,N-n); m = n \} \) if \( n = m \); and \( \Omega(n,m) = \{(n,m),(n,N-n),(N-n,m),(N-n,N-n),(m,n),(m,N-n),(N-m,n),(N-m,N-n) \} \) otherwise; follows from the fact that \( \cos \zeta_n + \cos \zeta_{m'} = \cos \zeta_n + \cos \zeta_{m'} \) when \((n',m') \in \Omega(n,m), \zeta_q = 2\pi q/N, q \in \{n,m\} \).

Thus from (11) we obtain
\[
\alpha_{|S,x,y;t|} = \frac{1}{N^2} \sum_{j=1}^{4N^2} [C_{r,j,1,0,0,k} (-1)^j + C_{r,j,2} + \sum_{n=1}^{N-1} \sum_{k=3}^{4} C_{r,j,n,0,k} \lambda_{n,0,k}^t + \sum_{n=1}^{N-1} \sum_{m=n+1}^{N-1} \sum_{k=3}^{4} C_{r,j,n,m,k} \lambda_{n,m,k}^t], 
\]
(14)
where
\[
C_{r,j,1} = \sum_{k=1,3,4} c_{r,j,0,0,k} + \sum_{n=1}^{N-1} c_{r,j,n,0,1} + \sum_{n=1}^{N-1} \sum_{m=n+1}^{N-1} c_{r,j,n,m,1}, \quad (15)
\]
\[
C_{r,j,2} = c_{r,j,0,0,2} + \sum_{n=1}^{N-1} c_{r,j,n,0,2} + \sum_{n=1}^{N-1} \sum_{m=n+1}^{N-1} c_{r,j,n,m,2}. \quad (16)
\]

Now we determine the time-averaged probability for the walker to be found at the initial position vertex \((0,0)\) with coin state \(|S'\rangle\) when the initial coin state of the walker is \(|S\rangle\) for the proposed DTQWs, \(S,S' \in \{R,L,U,D\}\).

First we have the following lemma which is easy to prove.

**Lemma 3.3.** Let \(\lambda_{n,m,k} \neq \lambda_{n',m',k'}\) be two eigenvalues of \(U\). Then
\[
\lim_{T \to \infty} \frac{1}{T} \sum_{t=0}^{T-1} (\lambda_{n,m,k})^t (\lambda_{n',m',k'})^t = 0.
\]

Then by Lemma 3.3 and equation (14), we obtain
\[
\mathcal{P}_N(S', (0,0); \psi_S(0)) = \frac{1}{N^4} \left[ \left( \sum_{j=1}^{4N^2} |C_{r,j,1}|^2 \right) + \left( \sum_{j=1}^{4N^2} |C_{r,j,2}|^2 \right) + \sum_{n=1}^{N-1} \sum_{k=1}^{4N^2} \sum_{j=1}^{4N^2} c_{r,j,n,0,k}|^2 + \sum_{n=1}^{N-1} \sum_{k=1}^{N-1} \sum_{j=1}^{N-1} c_{r,j,n,m,k}|^2 \right], \quad (17)
\]

**Remark 3.4.** (Dependence of \(\mathcal{P}_\infty(S', (0,0); \psi_S(0))\) on the constant eigenvalues of \(U\)) From equation \((17)\) it follows that the 3rd and 4th terms in the expression of \(\mathcal{P}_N(S', (0,0); \psi_S(0))\) are of order \(N^{-3}\), and the 5-th term is of order \(N^{-2}\). Thus all these terms vanish when \(N \to \infty\) and hence the probability of observing the walker at the vertex \((0,0)\), the initial position of the walker, depends only on the constant eigenvalues of the evolution operator \(U\) for the infinite lattice. Although for finite lattices, the time-averaged probability can be computed numerically using equation \((17)\), however it depends on the size of the lattice \(N^2\).

Thus for infinite lattice, the explicit formula for finding the walker with a coin state \(|S'\rangle\) for any initial canonical coin state \(|S\rangle\) can be obtained in terms of the entries of the eigenvectors corresponding to constant eigenvalues of \(U\) as follows.

\[
\mathcal{P}_\infty(S', (0,0); \psi_S(0)) = \lim_{N \to \infty} \mathcal{P}_N(S', (0,0); \psi_S(0)) \quad (18)
\]
\[
= \lim_{N \to \infty} \frac{1}{N^4} \left( |C_{r,j,1}|^2 + |C_{r,j,2}|^2 \right) = \frac{1}{N^4} \left( |C_{r,j,1}|^2 + |C_{r,j,2}|^2 \right),
\]
where \(S,S' \in \{R,L,U,D\}\) and \(r = l(S') + 2N^2 - 2, j = l(S) + 2N^2 - 2\).

Now we determine time-averaged probability for finding the walker on the infinite lattice at the initial position \((0,0)\) with coin state \(|S'\rangle\) when the initial coin state is \(|S\rangle\) and coin parameter \(\theta \in (-\pi, \pi), \theta \neq 0\).
Theorem 3.5. \( \overline{P}_\infty(S', (0,0); \psi_S(0)) = \frac{1}{8} \) if \( S = S' \in \{ R, L, U, D \} \), for \( \theta \neq 0, \pm \pi \).

Proof: Let \( |S\rangle = |S'\rangle = |R\rangle \). Note that, if \( |\varphi_S(0)\rangle = |\psi_S(0)\rangle \), \( 1 \leq j \leq 4N^2 \) then \( \psi_{2N^2-1}(0) = 1 \) and \( \psi_j(0) = 0 \) if \( j \neq 2N^2 - 1 \). Then by equations (15), (16) and (18) we have

\[
\overline{P}_\infty(R, (0,0); \psi_R(0)) = \lim_{N \to \infty} \frac{1}{N^4} \left( |C_{r,j,1}|^2 + |C_{r,j,2}|^2 \right)
\]

\[
= \lim_{N \to \infty} \frac{1}{N^4} \left( \sum_{j=1}^{N} \sum_{m=n+1}^{N} c_{r,j,n,m,1} + \sum_{j=1}^{N} \sum_{m=n+1}^{N} c_{r,j,n,m,2} \right)^2.
\]

\( r, j = 2N^2 - 1 \).

Clearly the constant and single summation terms in \( C_{r,j,1} \) and \( C_{r,j,2} \) vanishes while \( N \to \infty \) in the above expression. Now from Lemma 3.1 we have

\[
|v_{n,m,1}\rangle = \begin{bmatrix} (1 + \cos \theta + \sin \theta \omega^m)\omega^{-n} & - (1 + \cos \theta + \sin \theta \omega^m) \\ (1 + \cos \theta)\omega^{-n} + \sin \theta & (1 + \cos \theta)\omega^{-n} + \sin \theta \end{bmatrix}^{-1},
\]

\[
|v_{n,m,2}\rangle = \begin{bmatrix} (1 + \cos \theta - \sin \theta \omega^m)\omega^{-n} & (1 + \cos \theta - \sin \theta \omega^m) \\ (1 + \cos \theta)\omega^{-n} - \sin \theta & (1 + \cos \theta)\omega^{-n} - \sin \theta \end{bmatrix}^{-1},
\]

for \( \theta \neq 0, \pm \pi \). Thus using equation (13) we have \( c_{r,j,n,m,1} = c_{r,j,n,m,2} = 2 \). where \( r, j = 2N^2 - 1 \). Hence

\[
\overline{P}_\infty(R, (0,0); \psi_R(0)) = \lim_{N \to \infty} \frac{2}{N^4} \left( \sum_{n=1}^{N-3/2} \sum_{m=n+1}^{N-1/2} 2 \right)^2 = \lim_{N \to \infty} \frac{1}{N^4} \left( \frac{(N-1)(N-3)}{2} \right)^2 = \frac{1}{8}.
\]

Similarly the proof follows for other cases. \( \Box \)

Next we consider finding \( \overline{P}_\infty(S', (0,0); \psi_S(0)) \) when \( S \neq S' \). Indeed note that it ultimately boils down computing the constants \( c_{r,j,n,m,k} \) as follows. From equation (18) we have

\[
\overline{P}_\infty(S', (0,0); \psi_S(0)) = \lim_{N \to \infty} \frac{1}{N^4} \left( |C_{r,j,1}|^2 + |C_{r,j,2}|^2 \right)
\]

\[
= \lim_{N \to \infty} \frac{1}{N^4} \left( \sum_{n=1}^{N-3} \sum_{m=n+1}^{N-1} c_{r,j,n,m,1} + \sum_{n=1}^{N-3} \sum_{m=n+1}^{N-1} c_{r,j,n,m,2} \right)^2
\]

where \( S, S' \in \{ R, L, U, D \} \) and \( r = l(S') + 2N^2 - 2, j = l(S) + 2N^2 - 2 \). Now from equation (13) we have

\[
c_{r,j,n,m,k} = \sum_{(n',m') \in \Omega(n,m)} \frac{v_{l(S'),n',m',k}\overline{v}_{l(S),n',m',k}}{\|v_{n',m',k}\|^2}, k = 1, 2
\]

whose values can be obtained by placing the values of \( v_{l(S),n',m',k} \) and \( v_{l(S'),n',m',k} \) from Lemma 3.1, where \( r = l(S') + 2N^2 - 2 \) and \( j = l(S) + 2N^2 - 2, 1 \leq l(S), l(S') \leq 4 \). Indeed for \( \theta \neq 0, \pm \pi \),

\[
c_{r,j,n,m,1} = \begin{cases} 
-2 (\cos \zeta_n + \cos \zeta_m + 2 \sin \theta \cos \zeta_n \cos \zeta_m) & \text{if } \{ l(S), l(S') \} \in \{ \{1, 2\}, \{3, 4\} \}, l(S) \neq l(S'), \\
2 (1 + \cos \theta + (1 - \cos \theta) \cos \zeta_n \cos \zeta_m + \sin \theta (\cos \zeta_n + \cos \zeta_m)) & \text{if } l(S), l(S') \in \{ \{1, 3\}, \{2, 4\} \}, l(S) \neq l(S'), \\
-2 (\cos \zeta_n + \cos \zeta_m + \sin \theta \sin \theta \cos \zeta_n \cos \zeta_m) & \text{if } \{ l(S), l(S') \} \in \{ \{1, 4\}, \{2, 3\} \}, l(S) \neq l(S'), \\
2 ((1 + \cos \theta) \cos \zeta_n \cos \zeta_m + (1 - \cos \theta) + \sin \theta (\cos \zeta_n + \cos \zeta_m)) & \text{if } l(S), l(S') \in \{ \{2, 4\}, \{1, 3\} \}, l(S) \neq l(S'), \\
2 & \text{if } l(S), l(S') \in \{ \{1, 2, 3, 4\}, \{l(S) = l(S')\} \}, l(S) = l(S'),
\end{cases}
\]
\[ c_{r,j,n,m,k} = \begin{cases} \frac{2 \left( \cos \zeta_n + \cos \zeta_m - 2 \sin \theta \cos \zeta_n \cos \zeta_m \right)}{2 - \sin \theta \left( \cos \zeta_n + \cos \zeta_m \right)} & \text{if } \{l(S), l(S')\} \in \{\{1, 2\}, \{3, 4\}\}, l(S) \neq l(S') \\
\frac{2 (1 + \cos \theta + (1 - \cos \theta) \cos \zeta_n \cos \zeta_m - \sin \theta \cos \zeta_n \cos \zeta_m)}{2 (\cos \zeta_n + \cos \zeta_m)} & \text{if } \{l(S), l(S')\} \in \{\{1, 3\}, \{2, 3\}\}, l(S) \neq l(S') \\
\frac{2 (\cos \zeta_n + \cos \zeta_m - \sin \theta \cos \zeta_n \cos \zeta_m)}{2 - \sin \theta \left( \cos \zeta_n + \cos \zeta_m \right)} & \text{if } \{l(S), l(S')\} \in \{\{1, 4\}, \{2, 3\}\}, l(S) \neq l(S') \\
2 \left( \cos \zeta_n + \cos \zeta_m - 2 \sin \theta \cos \zeta_n \cos \zeta_m \right) & \text{if } l(S), l(S') \in \{1, 2, 3, 4\}, l(S) = l(S'). \\
\end{cases} \]

Observe that due to complicated expressions of \( c_{r,j,n,m,k} \), \( k = 1, 2 \) it is not feasible to come up with a value for \( \mathcal{P}_\infty(S'; (0, 0), \psi_S(0)) \) when \( S \neq S' \) for all \( \theta \in (-\pi, \pi) \), \( \theta \neq 0 \). However as \( N \to \infty \), the limiting value for the sum of \( c_{r,j,n,m,k} \) can be approximated by Riemann integration. For example, consider of \( c_{r,j,n,m,1} \) where \( l(S), l(S') \in \{1, 2, 3, 4\}, l(S) \neq l(S') \). Then,

\[
\lim_{N \to \infty} \frac{1}{N^2} \sum_{n=1}^{N-3} \sum_{m=n+1}^{N-1} c_{r,j,n,m,1} = \frac{1}{8\pi^2} \int_0^\pi \int_0^\pi \frac{-2(\cos x + \cos y + 2 \sin \theta \cos x \cos y)}{2 + \sin \theta (\cos x + \cos y)} dx \, dy.
\]

Then the total time-averaged probability for finding the walker at \((0, 0)\) is given by

\[
\mathcal{P}_\infty((0, 0); \psi_S(0)) = \sum_{S' \in \{R, L, U, D\}} \mathcal{P}_\infty(S', (0, 0); \psi_S(0))
\]

when the initial coin state of the walker is \( S \in \{R, L, U, D\} \), can be obtained after evaluating the Riemann integration for specific values of \( \theta, \theta \neq 0, \pm \pi \).

Following a similar process, for \( C \in Y_\theta \), \( \theta = 0, \pm \pi \) we evaluate that \( \mathcal{P}_\infty((0, 0); \psi_S(0)) = \frac{1}{8} \) for \( \theta = \pi, -\pi, S \in \{R, U\} \) or \( \theta = 0, S \in \{L, D\} \), and \( \mathcal{P}_\infty((0, 0); \psi_S(0)) = \frac{1}{4} \) for \( \theta = 0, S \in \{R, U\} \) or \( \theta = \pi, -\pi, S \in \{L, D\} \). In Figure 1 we plot \( \mathcal{P}_\infty((0, 0); \psi_S(0)) \) for different values of \( \theta \) obtained by discretizing the interval \([\theta \pi, \pi]\) into 400 equidistant points. Note that, if \( |\psi_S(0)| = |\psi_j(0)| \) then \( \psi_j(0) = 1 \) if \( j = l(S) + 2N^2 - 2 \) and 0 otherwise.

It follows from Figure 1 that the values of \( \mathcal{P}_\infty((0, 0); \psi_S(0)), S \in \{R, L, U, D\} \) corresponding to different \( \theta \) are symmetric with respect to the vertical axis passing through \( \theta = 0 \). Finally, we conclude that the proposed DTQWs with canonical initial coin states on infinite lattice localize when the initial position is \((0, 0)\). A similar analysis can be performed for any vertex \((x, y) \in \mathbb{Z} \times \mathbb{Z} \) as an initial position.
Remark 3.6. (Initial state correspond to $P_\infty(S', (0, 0); \psi(0)) = 0$) For the proposed quantum walks with an initial state $|\psi(0)\rangle$, using (11), (13) and (18) we obtain

$$P_\infty(S', (0, 0); \psi(0)) = \lim_{N \to \infty} \frac{1}{N^4} \left( \sum_{j=1}^{4N^2} C_{r,j,1}^2 + \sum_{j=1}^{4N^2} C_{r,j,2}^2 \right)$$

$$= \lim_{N \to \infty} \frac{1}{N^4} \left( \sum_{n=1}^{N-3} \sum_{m=1}^{N-1} \sum_{j=1}^{4N^2} C_{r,j,n,m,1}^2 + \sum_{n=1}^{N-3} \sum_{m=1}^{N-1} \sum_{j=1}^{4N^2} C_{r,j,n,m,2}^2 \right)$$

$$= \lim_{N \to \infty} \left( \sum_{n=0}^{N-1} \sum_{m=0}^{N-1} \eta_{r,n,m,1} \eta_{r,n,m,1}^* \langle \psi(0) \rangle^2 + \sum_{n=0}^{N-1} \sum_{m=0}^{N-1} \eta_{r,n,m,2} \eta_{r,n,m,2}^* \langle \psi(0) \rangle^2 \right),$$

where $r = l(S') + 2N^2 - 2$. Then it is clear that if the initial state $|\psi(0)\rangle$ is orthogonal to the eigenvectors $|\eta_{n,m,1}\rangle$, $|\eta_{n,m,2}\rangle$ corresponding to the eigenvalues $-1$ and $1$ of $U$, $0 \leq n, m \leq N - 1$, or in other words, if the eigenvectors $|\psi_{n,m,1}\rangle$, $|\psi_{n,m,2}\rangle$ are orthogonal to $|\psi_{0,0}(0)\rangle$ for all $(n, m)$, then $P_\infty(S', (0, 0); \psi(0)) = 0$ for $S' \in \{R, L, U, D\}$ and consequently $P_\infty((0, 0); \psi(0)) = 0$. Thus for such initial states, the walk does not localize at $(0, 0)$. A similar analysis can be done for any vertex $(x, y)$.

Now, in the following propositions we determine initial coin states which provide zero value of the total time-averaged probability.

Proposition 3.7. The walk with $C \in Y_\theta, \theta \in [-\pi, \pi]$, does not show localization at the initial position $(0, 0) \in \mathbb{Z} \times \mathbb{Z}$ if and only if the initial coin state $|\psi_{0,0}(0)\rangle \in I_0(y)$ where

$$I_0(y) = \left\{ [a, b, c, d]^T \in \mathbb{C}^4 | a = -c = \alpha(1 + \cos \theta), b = -d = -\alpha \sin \theta, \alpha \in \mathbb{C}, |\alpha|^2 = \frac{1}{4(1 + \cos \theta)} \right\}$$

if $\theta \notin \{0, \pm \pi\}$, $I_0(y) = \left\{ [\alpha, 0, -\alpha, 0]^T | \alpha \in \mathbb{C}, |\alpha|^2 = 1/2 \right\}$ if $\theta = 0$, and $I_0(y) = \left\{ [0, \alpha, 0, -\alpha]^T | \alpha \in \mathbb{C}, |\alpha|^2 = 1/2 \right\}$, if $\theta = \pm \pi$.

Proof: The ‘if’ part is easy to verify. The ‘only if’ part follows from Remark 3.6 that the initial coin state $|\psi_{0,0}(0)\rangle$ for which the underlying walk does not exhibit localization at $(0, 0)$ can be determined by considering that the following two conditions are satisfied

$$\langle v_{n,m,1}|\psi_{0,0}(0)\rangle = \langle v_{n,m,2}|\psi_{0,0}(0)\rangle = 0,$$

for each $(n, m), 0 \leq n, m \leq N - 1$. Thus by evaluating $|v_{n,m,1}\rangle$, $|v_{n,m,2}\rangle$ from Lemma 3.1 and Lemma 3.2, the desired results follows after performing some algebraic calculations. □

Clearly, by choosing initial state $|\psi_S(0)\rangle$, $S \in \{R, L, U, D\}$ for the walk with $C \in Y_\theta, \theta \in [-\pi, \pi]$ we obtain by Proposition 3.7 that $P_\infty((0, 0); \psi_S(0)) \neq 0$, which can be observed in Figure 1.

The theoretical results of Proposition 3.7 regarding the localization at $(0, 0)$ are illustrated numerically for some finite system size $N$ in Figure 2 and Figure 3 for the Grover walk and the walk with coin $C \in Y_\theta, \theta = \pi/6$, respectively. In each case we plot the probability distribution $P_t((x, y); \psi(0))$ after $t = 30$ time steps for two different types of initial coin states, one of which does not belong to $I_0(y)$ and another is taken from $I_0(y)$. When $|\psi_{0,0}(0)\rangle \notin I_0(y)$, we see that there are peaks in the probability distribution at the origin $(0, 0)$, while for $|\psi_{0,0}(0)\rangle \in I_0(y)$, the central peaks vanish and the probabilities spread symmetrically towards the other vertices.
In this section, we consider the proposed walks when the coin operator belongs to \( X_\theta \) or \( Z_\theta \), \([-\pi, \pi]\). If the coin operator \( C \in X_\theta \) then the walk evolution operator

\[
U'_{n,m} = D_{n,m}C = \begin{bmatrix}
\frac{1}{2} \sin \theta \omega^{-n} & -\frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} \sin \theta \omega^{m} & \frac{1}{2} (1 + \cos \theta) \omega^{-n} & \frac{1}{2} (1 + \cos \theta) \omega^{n} \\
\frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} (1 + \cos \theta) \omega^{n} & \frac{1}{2} (1 + \cos \theta) \omega^{-n} & \frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} \sin \theta \omega^{m} \\
\frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} \sin \theta \omega^{m} & \frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} (1 + \cos \theta) \omega^{-n} & \frac{1}{2} (1 + \cos \theta) \omega^{n} \\
\frac{1}{2} \sin \theta \omega^{m} & \frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} (1 + \cos \theta) \omega^{n} & \frac{1}{2} (1 + \cos \theta) \omega^{-n} \\
\frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} \sin \theta \omega^{m} & \frac{1}{2} (1 + \cos \theta) \omega^{-n} & \frac{1}{2} (1 + \cos \theta) \omega^{n} \\
\frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} \sin \theta \omega^{m} & \frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} (1 + \cos \theta) \omega^{n} & \frac{1}{2} (1 + \cos \theta) \omega^{-n}
\end{bmatrix}
\]

and if the coin operator \( C \in Z_\theta \) then the walk evolution operator

\[
U''_{n,m} = D_{n,m}C = \begin{bmatrix}
\frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} (1 + \cos \theta) \omega^{m} & \frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} (1 + \cos \theta) \omega^{-n} & \frac{1}{2} \sin \theta \omega^{m} \\
\frac{1}{2} (1 + \cos \theta) \omega^{n} & \frac{1}{2} \sin \theta \omega^{m} & \frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} (1 + \cos \theta) \omega^{-n} & \frac{1}{2} \sin \theta \omega^{m} \\
\frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} \sin \theta \omega^{m} & \frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} (1 + \cos \theta) \omega^{n} & \frac{1}{2} (1 + \cos \theta) \omega^{-n} \\
\frac{1}{2} \sin \theta \omega^{m} & \frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} (1 + \cos \theta) \omega^{n} & \frac{1}{2} (1 + \cos \theta) \omega^{-n} \\
\frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} \sin \theta \omega^{m} & \frac{1}{2} (1 + \cos \theta) \omega^{n} & \frac{1}{2} (1 + \cos \theta) \omega^{-n} \\
\frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} \sin \theta \omega^{m} & \frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} (1 + \cos \theta) \omega^{n} & \frac{1}{2} (1 + \cos \theta) \omega^{-n}
\end{bmatrix}
\]
where \(\theta \in [-\pi, \pi]\) and \(D_{n,m} = \text{diag}(\omega^{-n}, \omega^{n}, \omega^{-m}, \omega^{m})\), \(\omega = e^{2\pi i/N}\), \(m, n \in \{0, \ldots, N - 1\}\).

First we determine the eigenpairs of the unitary operators \(U'_{n,m}\) and \(U''_{n,m}\) as follows.

**Lemma 3.8.** A set of eigenpairs \((\lambda_{n,m,k}, |v'_{n,m,k}\rangle)\), \(k = 1, 2, 3, 4\) of \(U'_{n,m}\) are as follows. For \(\theta \neq 0, \pm \pi\),

\[
\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = \frac{\sin \theta (\cos \zeta_n + \cos \zeta_m) - i \sqrt{4 - \sin^2 \theta (\cos \zeta_n + \cos \zeta_m)^2}}{2},
\]

\[
\lambda_{n,m,4} = \frac{\sin \theta (\cos \zeta_n + \cos \zeta_m) + i \sqrt{4 - \sin^2 \theta (\cos \zeta_n + \cos \zeta_m)^2}}{2},
\]

\[
|v'_{n,m,k}\rangle = \left[ \sin \theta \omega^{-n}, \sin \theta \omega^{n}, \cos \theta \omega^{-m}, \cos \theta \omega^{m} \right]^T;
\]

for \(\theta = 0\),

\[
\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = -i, \lambda_{n,m,4} = i,
\]

\[
|v'_{n,m,k}\rangle = \left[ \lambda_{n,m,k} \omega^{-n}, \lambda_{n,m,k} \omega^{n}, \lambda_{n,m,k}^2 \omega^{-m}, \lambda_{n,m,k}^2 \omega^{m} \right]^T;
\]

and for \(\theta = \pm \pi\),

\[
\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = -i, \lambda_{n,m,4} = i,
\]

\[
|v'_{n,m,k}\rangle = \left[ \lambda_{n,m,k}^3 \omega^{-n}, \lambda_{n,m,k}^3 \omega^{n}, \lambda_{n,m,k}^2 \omega^{-m}, \lambda_{n,m,k}^2 \omega^{m} \right]^T;
\]

where \(\omega = e^{2\pi i/N}\).

**Proof:** The proof follows from the fact that the characteristic polynomial of \(U'_{n,m}\) is

\[
\chi_{U'_{n,m}}(\lambda) = \lambda^4 - \sin(\theta(\cos \zeta_m + \cos \zeta_n))\lambda^3 + \sin(\theta(\cos \zeta_m + \cos \zeta_n))\lambda - 1.
\]

\[\Box\]

**Lemma 3.9.** A set of eigenpairs \((\lambda_{n,m,k}, |v''_{n,m,k}\rangle)\), \(k = 1, 2, 3, 4\) of \(U''_{n,m}\) are given as follows. For \(\theta \neq 0, \pm \pi\),

\[
\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = \frac{\sin \theta (\cos \zeta_n + \cos \zeta_m) - i \sqrt{4 - \sin^2 \theta (\cos \zeta_n + \cos \zeta_m)^2}}{2},
\]

\[
\lambda_{n,m,4} = \frac{\sin \theta (\cos \zeta_n + \cos \zeta_m) + i \sqrt{4 - \sin^2 \theta (\cos \zeta_n + \cos \zeta_m)^2}}{2},
\]

\[
|v''_{n,m,k}\rangle = \left[ \frac{\sin \theta (1 + \cos \theta)(\lambda_{n,m,k} \omega^{-n})}{(1 + \cos \theta) - \lambda_{n,m,k} \sin \theta \omega^{-n}}, \frac{\sin \theta (1 + \cos \theta)(\lambda_{n,m,k} \omega^{n})}{(1 + \cos \theta) - \lambda_{n,m,k} \sin \theta \omega^{n}}, \sin \theta (1 + \cos \theta)(\lambda_{n,m,k} \omega^{-m}) \right]^T;
\]

for \(\theta = 0\),

\[
\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = -i, \lambda_{n,m,4} = i,
\]

\[
|v''_{n,m,k}\rangle = \left[ \lambda_{n,m,k}^2 \omega^{-n}, \lambda_{n,m,k}^3 \omega^{n}, \lambda_{n,m,k} \omega^{-m}, \lambda_{n,m,k} \omega^{m} \right]^T;
\]
and for $\theta = \pm \pi$,
\[
\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = -i, \lambda_{n,m,4} = i,
\]
\[
|v''_{n,m,k}\rangle = [\lambda_2^{n,m,k}\omega^{-n-m}, \lambda_{n,m,k}\omega^{-m}, \lambda_3^{n,m,k}\omega^{-m}, 1]^T;
\]
where $\omega = e^{2\pi i/N}$.

**Proof:** The proof follows from the fact that the characteristic polynomial of $U''_{n,m}$ is
\[
\chi(U''_{n,m})(\lambda) = \lambda^4 - \sin \theta (\cos \zeta_n + \cos \zeta_m)\lambda^3 + \sin \theta (\cos \zeta_m + \cos \zeta_n)\lambda - 1.
\]

Note that $\Lambda(U_{n,m}) = \Lambda(U'_n,m) = \Lambda(U''_{n,m})$. Besides, a set of orthonormal eigenvectors of the evolution matrix corresponding to the DTQWs defined by generalized Grover coins in $X_\theta$ and $Z_\theta$ can be obtained by employing similar arguments as in the previous section. Thus an integration formula of time-average probabilities can be determined for these walks. Indeed, recall from (18) that
\[
P_\infty(S', (0,0); \psi_S(0)) = \lim_{N \to \infty} \frac{1}{N^4} \left( \sum_{n=1}^{(N-3)/2} \sum_{m=n+1}^{(N-1)/2} c_{r,j,n,m,1}^2 + \sum_{n=1}^{(N-3)/2} \sum_{m=n+1}^{(N-1)/2} c_{r,j,n,m,2}^2 \right),
\]
$S' \in \{R, L, U, D\}$. The values of $c_{r,j,n,m,k}, k = 1, 2$ can be calculated using equation (13).

It may be noted that explicit expressions of $c_{r,j,n,m,k}, k = 1, 2$ for different $r$ and $j$ is complicated. Thus we perform numerical computations for the values of $P_\infty((0,0); \psi_S(0))$ for different values of $\theta$. We find that $c_{r,j,n,m,k}$ are same for some pairs $(r,j)$, for example $c_{1,3,n,m,k} = c_{1,4,n,m,k} = c_{2,3,n,m,k} = c_{2,4,n,m,k} = c_{3,1,n,m,k} = c_{3,4,n,m,k} = c_{4,1,n,m,k} = c_{4,2,n,m,k} = c_{4,3,n,m,k} = c_{4,4,n,m,k}$ which finally results in $P_\infty((0,0); \psi_S(0))$ to be same for all $S \in \{R, L, U, D\}$ since $c_{r,j,n,m,k} = c_{j,r,n,m,k}$, when the coin operator belongs to $X_\theta$.

We plot $P_\infty((0,0); \psi_R(0))$ considering 400 equidistant values of $\theta$ in the interval $[-\pi, \pi]$ in Figure 4. It can be further observed from Figure 4 that the probability distribution $P_\infty((0,0); \psi_R(0))$ is symmetric with respect to the vertical axis through $\theta = 0$. Probabilities are maximum at $\theta = \pi/2, -\pi/2$ i.e. coin operators are $G, P_{(12)(34)}G$ and minimum at $\theta = 0, \pi, -\pi$ i.e. coin operators are $P_{(1324)}, P_{(1423)}$. Finally, we conclude the proposed walks corresponding to these values of the coin parameter $\theta$ with the initial state $\psi_S(0), S \in \{R, L, U, D\}$ localize at the initial position $(0,0)$ of the infinite lattice.

![Figure 4: Numerical values of $P_\infty((0,0); \psi_S(0)), S \in \{R, L, U, D\}$ when the coins belong to $X_\theta$ with 400 equidistant values of $\theta$ in $[-\pi, \pi]$.](image)

In the next proposition we show that the proposed walks with $C \in X_\theta, \theta \in [-\pi, \pi], \theta \neq -\frac{\pi}{2}$ i.e. $C \neq G$, show localization at initial position for any initial coin state.
Proposition 3.10. The walk with $C \in X_\theta, \theta \in [-\pi, \pi], \theta \neq -\frac{\pi}{2}$ shows localization at the position $(0, 0) \in \mathbb{Z} \times \mathbb{Z}$ for any initial coin state.

Proof: First consider the case for $\theta = 0$. Then by Lemma 3.8 the eigenvectors of $U'_{n,m}$ corresponding to the eigenvalues $-1$ and $1$ are

$$|v'_{n,m,1}\rangle = [\omega^{n-m}, -\omega^n, \omega^{n-m}, 1]^T$$ and $$|v'_{n,m,2}\rangle = [\omega^{n-m}, \omega^n, \omega^{n-m}, 1]^T.$$ Next for $\theta = \pm \pi$ we have

$$|v'_{n,m,1}\rangle = [\omega^{-m}, -\omega^{-m}, -\omega^{-m}, 1]^T$$ and $$|v'_{n,m,2}\rangle = [\omega^{-m}, \omega^{-m}, \omega^{-m}, 1]^T.$$ Finally, for $\theta \neq 0, \pm \pi$, we recall $|v'_{n,m,1}\rangle$ and $|v'_{n,m,2}\rangle$ from Lemma 3.8. Then by using Remark 3.6, the proof follows from the fact that there does not exist any initial coin state which is orthogonal to both $|v'_{n,m,1}\rangle$ and $|v'_{n,m,2}\rangle$ for each $n, m$ where $0 \leq n, m \leq N - 1$.

Next we plot the total time-averaged probabilities in Figure 5 for canonical initial coin states when the coin operator is in $Z_\theta$, for different values of $\theta$ obtained by discretizing the interval $[-\pi, \pi]$ into 400 equidistant points. Observe that, $\overline{P}_\infty((0, 0); \psi_S(0)), S \in \{R, L, U, D\}$ are symmetric with respect to the vertical axis $\theta = 0$ and the time-averaged probability decreases or increases depending on the initial coin state when $|\theta|$ increases. Obviously, the DTQWs defined by these generalized Grover coins with the canonical initial coin states localize at the vertex $(0, 0)$ of the infinite lattice.

![Figure 5: Numerical values of $\overline{P}_\infty((0, 0); \psi_S(0)), S \in \{R, L, U, D\}$ when the coins belong to $Z_\theta$ for 400 equidistant values of $\theta$ in $[-\pi, \pi]$.](image)

In following proposition we determine all the initial coin states for which the walks do not exhibit localization when the coin operator $C \in Z_\theta$.

Proposition 3.11. The walk with $C \in Z_\theta, \theta \in [-\pi, \pi]$, does not show localization at the initial position $(0, 0) \in \mathbb{Z} \times \mathbb{Z}$ if and only if the initial coin state $|\psi_{0,0}(0)\rangle \in I_0^{(z)}$ where

$$I_0^{(z)} = \left\{ [a, b, c, d]^T \in \mathbb{C}^4 | a = -d = \alpha(1 + \cos \theta), b = c = -\alpha \sin \theta, \alpha \in \mathbb{C}, |\alpha|^2 = \frac{1}{4(1 + \cos \theta)} \right\}$$ if $\theta \notin \{0, \pm \pi\}$, $I_0^{(z)} = \{ [\alpha, 0, 0, -\alpha]^T | \alpha \in \mathbb{C}, |\alpha|^2 = 1/2 \}$ if $\theta = 0$, and $I_0^{(z)} = \{ [0, \alpha, -\alpha, 0]^T | \alpha \in \mathbb{C}, |\alpha|^2 = 1/2 \}$, if $\theta = \pm \pi$.

Proof: The proof follows similarly as Propositions 3.7 by using Lemma 3.9. □

Note that, by Proposition 3.11, if the walk is defined for the coin $C \in Z_\theta$ and the initial state is $|\psi_S(0)\rangle, S \in \{R, L, U, D\}$, we obtain $\overline{P}_\infty((0, 0); \psi_S(0)) \neq 0, \theta \in [-\pi, \pi]$.  

15
3.3 With coins from $W_\theta$

In this section, we consider the proposed walks when the coin operator lies in $W_\theta$, $\theta \in [-\pi, \pi]$. As mentioned before, note that $W_\theta$ does not contain the Grover matrix and hence this set of parametric coins need not be treated as continuous deformation of the Grover matrix. We demonstrate that the total probability value of these walks with initial coin state $|\psi_S(0)\rangle$ approaches to zero when $S \in \{R, L\}$ and $\theta \to 0$, and $S \in \{U, D\}$ and $\theta \to \pm \pi$.

Let $C \in W_\theta$. Then the walk evolution operator is given by

$$U''_{n,m} = D_{n,m}C = \begin{bmatrix}
\frac{1}{2}(1 + \cos \theta)\omega^n & \frac{1}{2}(1 - \cos \theta)\omega^{-n} & \frac{1}{2}\sin \theta\omega^n & -\frac{1}{2}\sin \theta\omega^{-n} \\
\frac{1}{2}\sin \theta\omega^n & \frac{1}{2}(1 + \cos \theta)\omega^n & \frac{1}{2}(1 - \cos \theta)\omega^{-n} & \frac{1}{2}(1 + \cos \theta)\omega^{-n} \\
-\frac{1}{2}\sin \theta\omega^{-m} & -\frac{1}{2}\sin \theta\omega^m & \frac{1}{2}(1 - \cos \theta)\omega^n & \frac{1}{2}(1 - \cos \theta)\omega^{-n} \\
\frac{1}{2}(1 - \cos \theta)\omega^m & \frac{1}{2}(1 + \cos \theta)\omega^{-m} & -\frac{1}{2}\sin \theta\omega^m & \frac{1}{2}\sin \theta\omega^{-m}
\end{bmatrix}$$

for $-\pi \leq \theta \leq \pi, \omega = e^{2\pi i/N}$, $m, n \in \{0, \ldots, N - 1\}$. Now we determine a set of eigenvectors of $U''_{n,m}$ in the following lemma.

**Lemma 3.12.** A set of eigenpairs $(\lambda_{n,m,k}, |v''_{n,m,k}\rangle)$, $k = 1, 2, 3, 4$ of $U''_{n,m}$ are given as follows. For $\theta \neq 0, \pm\pi$,

$$\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = e^{i\eta}, \lambda_{n,m,4} = e^{-i\eta},$$

where $\cos \eta = \frac{(1 + \cos \theta) \cos \zeta_n + (1 - \cos \theta) \cos \zeta_{m,n} - 1}{2}$.

$$|v''_{n,m,k}\rangle = \begin{bmatrix}
\sin(1 - \lambda_{n,m,k}\omega^m) \\
\sin(1 - \lambda_{n,m,k}\omega^{-m}) \\
\sin(1 - \lambda_{n,m,k}\omega^m)
\end{bmatrix}
\begin{bmatrix}
1 \\
1 \\
1
\end{bmatrix}
\begin{bmatrix}
1 - \lambda_{n,m,k}\omega^m \\
1 - \lambda_{n,m,k}\omega^{-m}
\end{bmatrix}^T$$

for $\theta = 0$,

$$\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = \omega^{-n}, \lambda_{n,m,4} = \omega^n,$$

$$|v''_{n,m,1}\rangle = \begin{bmatrix} 0, 0, \omega^{-m}, 1 \end{bmatrix}^T, |v''_{n,m,2}\rangle = \begin{bmatrix} 0, 0, \omega^{-m}, 1 \end{bmatrix}^T,$$

$$|v''_{n,m,3}\rangle = \begin{bmatrix} 1, 0, 0, 0 \end{bmatrix}^T, |v''_{n,m,4}\rangle = \begin{bmatrix} 0, 1, 0, 0 \end{bmatrix}^T;$$

and for $\theta = \pm\pi$,

$$\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = \omega^{-m}, \lambda_{n,m,4} = \omega^n,$$

$$|v''_{n,m,1}\rangle = \begin{bmatrix} -\omega^{-n}, 1, 0, 0 \end{bmatrix}^T, |v''_{n,m,2}\rangle = \begin{bmatrix} \omega^{-n}, 1, 0, 0 \end{bmatrix}^T,$$

$$|v''_{n,m,3}\rangle = \begin{bmatrix} 0, 0, 1, 0 \end{bmatrix}^T, |v''_{n,m,4}\rangle = \begin{bmatrix} 0, 0, 1, 0 \end{bmatrix}^T;$$

where $\omega = e^{2\pi i/N}$.

**Proof:** The characteristic polynomial of $U''_{n,m}$ is

$$\chi_{U''_{n,m}}(\lambda) = \lambda^4 - (\cos \zeta_n + \cos \zeta_m + \cos \zeta_n \cos \theta - \cos \zeta_m \cos \theta) \lambda^3 + (\cos \zeta_m + \cos \zeta_n + \cos \zeta_n \cos \theta - \cos \zeta_m \cos \theta) \lambda^2 - 1.$$

Solving $\chi_{U''_{n,m}}(\lambda) = 0$ we get the required eigenvalues.

Adapting similar procedures as in the above subsections, the values of total time-averaged probabilities $\overline{P}_\infty((0,0);\psi_S(0))$, $S \in \{R, L, U, D\}$ can be determined numerically for canonical initial coin states for infinite lattice. In Figure 6, we plot $\overline{P}_\infty((0,0);\psi_S(0))$ for different values of $\theta$ obtained by discretizing the interval $[-\pi, \pi]$ into 400 equidistant points. Then observe that the total probabilities are symmetric about the vertical axis through $\theta = 0$, where it becomes zero for initial coin state $|\psi_S(0)\rangle$, $S \in \{R, L\}$. Indeed, $\overline{P}_\infty((0,0);\psi_S(0))$ increases and decreases as $|\theta|$ increases for $S \in \{R, L\}$ and $S \in \{U, D\}$, respectively. Besides, observe that the total probabilities $\overline{P}_\infty((0,0);\psi_S(0))$, $S \in \{U, D\}$ approach to zero for several coins when $|\theta|$ equals to $\pi$.  

16
In following proposition we determine the initial coin states for which the proposed quantum walks give the total time-averaged probability zero when $C \in W_\theta$.

**Proposition 3.13.** The walk with $C \in W_\theta, \theta \in [-\pi, \pi]$, does not show localization at the initial position $(0, 0) \in \mathbb{Z} \times \mathbb{Z}$ if and only if the initial coin state $|\psi_{0,0}(0)\rangle \in I_0^{(w)}$ where

$$I_0^{(w)} = \left\{ [a,b,c,d]^T \in \mathbb{C}^4 | a = b = \alpha (1 + \cos \theta), c = -d = \alpha \sin \theta, \alpha \in \mathbb{C}, |\alpha|^2 = \frac{1}{4(1 + \cos \theta)} \right\}.$$  

if $\theta \notin \{0, \pm \pi\}$, $I_0^{(w)} = \{ [\alpha, \beta, 0, 0]^T | \alpha, \beta \in \mathbb{C}, |\alpha|^2 + |\beta|^2 = 1 \}$ if $\theta = 0$, and $I_0^{(w)} = \{ [0, 0, 0, 0]^T | \alpha, \beta \in \mathbb{C}, |\alpha|^2 + |\beta|^2 = 1 \}$, if $\theta = \pm \pi$.

**Proof:** The proof follows similarly as Proposition 3.7, by using Lemma 3.12. \qed

Note that, for the walk with $C \in W_\theta$ we obtain $T_\infty^{(0,0)}|\psi_S(0)\rangle = 0$, for $S \in \{R, L\}$ when $\theta = 0$ and $S \in \{U, D\}$ when $\theta = \pm \pi$ by Proposition 3.13. These results can be observed in Figure 6.

**Remark 3.14.** From Remark 3.4 and 3.6, it follows that localization property of the proposed quantum walks on infinite lattice depends on the constant eigenvalues of the evolution operator, and if initial state belongs to the orthogonal complement of the eigenspaces corresponding to the constant eigenvalues then the walks do not localize at the initial position, which is also established in [18] for periodic evolution operator and speculated in several other articles. The framework of investigating the asymptotic behavior of quantum walks on a finite lattice and then extending it to infinite lattice helps deriving a computable formula for the total time-averaged probability of finding the walker at its initial position for infinite lattice. The technique of approximating the probability amplitudes of the quantum state of the walker through an integral formula enables us to calculate the total time-averaged probability in terms of the coin parameter $\theta$. This reveals how the total time-averaged probability depends on the coin parameter that can be used for specific applications.

**Conclusion.** In this paper, we study discrete-time four-state quantum walks on two-dimension lattices. The coins are considered as one-parameter orthogonal matrices that are also permutative, a property of the Grover matrix. We focus on four sets of parametric coins denoted as $X_0, Y_0, Z_0$ and $W_\theta$ such that the Grover matrix belongs to the first three classes for some value of $\theta$. We perform a thorough analysis of localization phenomena of these walks. We
show that walks with coin operators from $X_\theta, Y_\theta$ and $Z_\theta$ localize at the initial position of the walker, which is considered as the origin of the two-dimensional lattices, for canonical initial coin states. However, this does not hold true for all coins in $W_\theta$. We also show that for coins in $X_\theta, \theta \neq \pi/2$ the walks localize for any initial coin state, whereas we provide a complete characterization of initial coin states for walks with coins from $Y_\theta, Z_\theta, W_\theta$ for which the corresponding walks do not localize at the initial position.

Acknowledgement. Amrita Mandal thanks Council for Scientific and Industrial Research (CSIR), India for financial support in the form of a junior/senior research fellowship. Rohit Sarma Sarkar acknowledges support through Prime Minister Research Fellowship (PMRF), Government of India.

References

[1] Bataille, M., Quantum circuits of CNOT gates: optimization and entanglement, *Quantum Information Processing* 21, no 7, 1–33 (2022).

[2] Higuchi, Yusuke and Konno, Norio and Sato, Iwao and Segawa, Etsuo, Spectral and asymptotic properties of Grover walks on crystal lattices, *Journal of Functional Analysis* 267, no. 11, 4197–4235 (2014).

[3] Inui, N., Konishi, Y., Konno, N., Localization of two-dimensional quantum walks, *Physical Review A* 69, no. 5, 052323 (2004).

[4] Inui, N., Konno, N., Localization of multi-state quantum walk in one dimension, *Physica A: Statistical Mechanics and its Applications* 353, 133–144 (2005).

[5] Kollár, B., Kiss T., Jex, I., Strongly trapped two-dimensional quantum walks, *Physical Review A* 91, no. 2, 022308 (2015).

[6] Kollár, B., Gilyén, A., Tkáčová, I., Kiss, T., Jex, I., Štefaňák, M., Complete classification of trapping coins for quantum walks on the two-dimensional square lattice, *Physical Review A* 102, no. 1, 012207, (2020).

[7] Komatsu, T., Tate, T., Eigenvalues of quantum walks of Grover and Fourier types, *Journal of Fourier Analysis and Applications* 25, no. 4, 1293–1318 (2019).

[8] Konno, N., Localization of an inhomogeneous discrete-time quantum walk on the line, *Quantum Information Processing* 9, 405–418 (2010).

[9] Lyu, C., Yu, L., Wu, S., Localization in quantum walks on a honeycomb network, *Physical Review A* 92, no. 5, 052305 (2015).

[10] Machida T., Limit theorems of a 3-state quantum walk and its application for discrete uniform measures, *Quantum Information and Computation, Vol.15 No.5 & 6*, 406-418 (2015).

[11] Machida T., A limit law of the return probability for a quantum walk on a hexagonal lattice, *International Journal of Quantum Information, Vol.13, No.7*, 1550054 (2015).

[12] Machida, T., Chandrashekar C.M., Localization and limit laws of a three-state alternate quantum walk on a two-dimensional lattice, *Physical Review A*, 92, 062307 (2015).

[13] Mandal, A., Adhikari, B., A characterization of orthogonal permutative matrices of order 4, *Linear Algebra and its Applications* 654, 102-124 (2022).
[14] Mandal, A., Sarkar, R.S., Chakraborty, S. and Adhikari, B., Limit theorems and localization of three state quantum walks on a line defined by generalized Grover coins, \textit{arXiv preprint arXiv:2204.05625}, (2022).

[15] Sarma Sarkar, R., Mandal, A., Adhikari, B., Periodicity of lively quantum walks on cycles with generalized Grover coin, \textit{Linear Algebra and its Applications 604}, 399–424 (2020).

[16] Segawa, E., Suzuki, A., Generator of an abstract quantum walk, \textit{Quantum Studies: Mathematics and Foundations 3}, no. 1, 11–30 (2016).

[17] Štefaňák, M., Bezděková, I., Jex, I., Continuous deformations of the Grover walk preserving localization, \textit{The European Physical Journal D 66}, no. 5, 142 (2012).

[18] Tate, T., Eigenvalues, absolute continuity and localizations for periodic unitary transition operators \textit{Infinite Dimensional Analysis, Quantum Probability and Related Topics 22}, no. 02, 1950011 (2019).

[19] Tregenna, B., Flanagan, W., Maile, R., Kendon, V., Controlling discrete quantum walks: coins and initial states, \textit{New Journal of Physics 5}, no. 1, 83 (2003).

[20] Venegas A., Salvador E., Quantum walks: a comprehensive review, \textit{Quantum Information Processing 11}, no. 5, 1015-1106 (2012).

[21] Watabe, K., Kobayashi, N., Katori, M., Konno, N., Limit distributions of two-dimensional quantum walks, \textit{Physical Review A 77}, no. 6, 062331 (2008).

[22] Wojcik, A., Luczak, T., Kurzynski, P., Grudka, A., Gdala, T., Bednarska-Bzdęga, M., Trapping a particle of a quantum walk on the line, \textit{Physical Review A 85}, no. 1, 012329 (2012).
Localization of two-dimensional quantum walks defined by generalized Grover coins

Amrita Mandal∗, Rohit Sarma Sarkar†, Bibhas Adhikari‡

Abstract. In this paper, we study the localization phenomena of discrete-time coined quantum walks (DTQWs) on two-dimensional lattices when the coins are permutative orthogonal (real) matrices of order $4 \times 4$. First, we provide a complete characterization of all complex, real and rational permutative orthogonal matrices of dimension $4 \times 4$, and consequently we determine new chains of groups of orthogonal matrices. Next, we determine matrix spaces generated by certain permutation matrices of order $4 \times 4$ such that orthogonal matrices in these spaces are permutative matrices or direct sum of permutative matrices up to permutation of rows and columns. However, we provide an example of a matrix space which contains orthogonal matrices that are neither of these forms. Then we establish that the localization phenomena of Grover walk at initial position corresponding to canonical initial coin states is extended to the proposed quantum walks on two-dimensional infinite lattice with generalized Grover coins, which need not be true for any coin which is a permutative orthogonal (real) matrix.

Keywords. Quantum walk, permutative matrix, Grover matrix

AMS subject classification(2000): 81S25, 05C38, 15B10

1 Introduction

Quantum walks are quantum analogue of classical random walks and it constitute universal models of quantum computation [4], [16], [5]. The feature of ballistic spread of probability distribution of the quantum walker makes quantum walks strikingly different from their classical counterpart [33]. Quantum walks, in particular two-dimensional quantum walks are successfully realized experimentally in [27], [23], [28]. There are two models of quantum random walks based on either discrete-time steps or continuous-time evolution [30]. In this paper, we consider Discrete-time quantum walks (DTQWs) on two-dimensional lattices.

DTQWs on graphs are defined in terms of repeated application of a unitary operator $U = S_f(C \otimes I)$ to the initial state of the walker, where $S_f$ is called the shift operator and $C$ is called coin operator. The operator $U$ acts on the Hilbert space $\mathcal{H}_p \otimes \mathcal{H}_c$ where $\mathcal{H}_p$ defines the position space spanned by the quantum states localized at the vertices of the graph, and $\mathcal{H}_c$ defines the coin space whose dimension gives the internal degree of freedom of the quantum coin associated with the quantum walk. Here $\otimes$ denotes the tensor product of vector spaces. Thus, like the classical case, a quantum walker in a quantum walk moves to another vertex defined by the shift operator conditional to the coin state of the present position, however the coin state can be in the superposition of canonical coin states.

Obviously, the behavior of a DTQW depends on the choice of the coin operator [2]. The Grover diffusion matrix, which was first utilized by Grover in [9] for the Grover search algorithm is a popular choice for the coin operator in literature for DTQWs on graphs [11], [7], [18], [10]. A quantum walk is also called Grover walk when the coin operator of the walk is

∗Department of Mathematics, IIT Kharagpur, Email: mandalamrita55@gmail.com
†Department of Mathematics, IIT Kharagpur, Email: rohit15sarkar@yahoo.com
‡Corresponding author, Department of Mathematics, IIT Kharagpur, Email: bibhas@maths.iitkgp.ac.in
the Grover matrix. Grover walk is generalized in literature by generalizing the Grover matrix into a class of parametric unitary matrices [31]. In [25], the parametric coin operators are proposed using projectors corresponding to the eigenvectors of the Grover matrix.

An interesting but obvious observation is that Grover matrix is a permutative orthogonal matrix, that is, an orthogonal matrix whose every row is a permutation of any other row [22]. Hence Grover walk can be generalized by considering the coin operators as permutative orthogonal matrices that can help an improved understanding of the underlying quantum dynamics and how it differs from its classical counterpart. Besides, a parametric representation of all such matrices can give insights about how the behavior of such quantum walks are influenced by the values of the parameters that should be suitable for specific applications. For instance, localization is an uncommon property of certain quantum walks in which the walker can be found at a vertex such as initial position with nonzero probability even if the number of steps approaches to infinity [15], [30]. This phenomena is also called the walker’s localization. This is observed in [29] for the first time for the numerical investigation of Grover walk on two-dimensional square lattices. Localization phenomena makes a walk overwhelmingly different since in classical random walks on a line or a square lattice, the probability of finding the walker at a specific position approaches zero when the number of steps is large enough. Indeed, localization is found in several quantum walks defined by different coin operators, see [10], [11], [14], [17], [32] and the references therein. Thus it would be of paramount interest to investigate localization property of DTQWs defined by generalized Grover coin operators on square or infinite lattices.

In this paper, first we determine parametric representation of all complex orthogonal matrices of order $4 \times 4$ that are permutative. Consequently, we determine chains of matrix subgroups of $4 \times 4$ complex orthogonal matrices. Further, we are able to derive one-parameter representation of all real and rational permutative orthogonal matrices of order $4 \times 4$. We identify the classes of those one-parameter matrices which include the Grover matrix as a special case and we call these matrices as generalized Grover matrices. These matrices can act as four dimensional coin operators for DTQWs on graphs. We also show that permutative orthogonal matrices of order $4 \times 4$ are linear sum of permutation matrices. It is observed before that an orthogonal matrix of order $3 \times 3$ is permutative if and only if it is a linear sum of permutation matrices [22]. In this paper we show that this is no longer true for $n = 4$. We show that any linear sum of two or three permutations matrices is either permutative or direct sum of permutative matrices up to permutation of rows and columns, if they are orthogonal.

Then we extend our study with a suitable choice of a maximal linearly independent set of permutation matrices of order $4 \times 4$ to determine classes of non-permutative orthogonal matrices of order $4 \times 4$. Consequently, we identify matrix spaces generated by permutations that orthogonal matrices in these spaces are permutative, direct sum of permutative up to permutations of rows and columns or neither of these forms. We mention that this characterization has implications to solving the open problem of characterizing all orthogonal matrices that are linear sum of permutations matrices, a problem of interest in quantum computing community [13].

Next we define DTQWs on two-dimensional lattices that are defined by coin operators which are real permutative orthogonal matrices. Then we investigate the localization property of these DTQWs which generalizes the study of Inui et al. of Grover walk on square and infinite lattices [10]. We show that the localization property of Grover walk on infinite lattice extends to the proposed DTQWs for canonical initial coin states with generalized Grover coins. Thus we show that the walker can be found at the initial position which is the vertex $(0,0)$ of the infinite lattice, with a nonzero total time-averaged probability. This phenomena is also called trapping of the walker [14]. Further, we show that the localization property as observed for generalized Grover coins need not extend to classes of orthogonal matrices which are permutative orthogonal but do not belong to the classes of generalized Grover coins. Then we demonstrate that the total time-averaged probability of finding the walker at initial
position tends to zero for several coins that are permutative matrices but not generalized Grover matrices.

The organization of this paper is as follows. In Section 2 we provide a complete characterization of complex, real and rational permutative matrices of order $4 \times 4$. We determine chains of groups of permutative orthogonal matrices. In Section 3 we investigate the localization phenomena of the proposed DTQWs and we establish that the localization property of Grover walk extends to these generalized Grover walks on infinite lattices for initial canonical coin states. Finally, we consider the proposed DTQWs defined by a class of coins that are permutative but do not lie in the classes of generalized Grover coins, and we show that localization property at the initial position is not observed for several such coins when the initial coin states are canonical.

2 Permutative orthogonal matrices of order $4 \times 4$

Recall that a matrix is called permutative if any of its row is a permutation of any other row [20]. Thus, such a matrix of order $n \times n$ has $n$ parameters in its symbolic form. Without loss of generality, a permutative matrix of order $4 \times 4$ can be written in the symbolic form

$$A(x; P, Q, R) = \begin{bmatrix} x \\ xP \\ xQ \\ xR \end{bmatrix}$$

where $x = [x \ y \ z \ w]$ is a symbolic row vector with $x, y, z, w \in \mathbb{C}$ and $P, Q, R \in \mathcal{P}_4$, the group of permutation matrices of order $4 \times 4$ [19]. Let $S_4$ denote the symmetric group on 4 elements. If $\pi \in S_4$ then the permutation matrix corresponding to $\pi$ is defined as $P_\pi = [p_{ij}]$ where $p_{ij} = 1$ if $\pi(i) = j$, and $p_{ij} = 0$ otherwise. A permutative orthogonal matrix is a matrix that is both permutative and orthogonal, for example, any permutation matrix is a permutative orthogonal matrix. Let $\mathcal{PO}_4$ denote the set of all permutative orthogonal matrices of order $4 \times 4$. Then obviously $\mathcal{P}_4 \subset \mathcal{PO}_4$. We denote $1 \oplus \mathcal{P}_3 = \{ [1 \ 0^T \ 0] \in \mathcal{P}_4 : P \in \mathcal{P}_3 \}$, where $0 = [0 \ 0 \ 0]^T$ and $\mathcal{P}_3$ denotes the group of all permutation matrices of order $3 \times 3$.

Then the following theorem characterizes all matrices in $\mathcal{PO}_4$.

**Theorem 2.1.** A matrix $A$ of order $4 \times 4$ is permutative (complex) orthogonal if and only if $A \in \mathcal{X} \cup \mathcal{Y} \cup \mathcal{Z}$ where

$$\mathcal{X} = \{ PM_{x,z}, PN_{x,z}^\pm : x^2 + z^2 \mp z = 0, x, z \in \mathbb{C} \}$$

$$\mathcal{Y} = \{ PP_{(23)}M_{x,z}^\pm P_{(23)}, PP_{(23)}N_{x,z}^\pm P_{(23)} : x^2 + z^2 \mp z = 0, x, z \in \mathbb{C} \}$$

$$\mathcal{Z} = \{ PP_{(24)}M_{x,z}^\pm P_{(24)}, PP_{(24)}N_{x,z}^\pm P_{(24)} : x^2 + z^2 \mp z = 0, x, z \in \mathbb{C} \}$$

where

$$M_{x,z}^\pm = \begin{bmatrix} A_x & B_x^\pm \\ B_x^\pm & -A_x \end{bmatrix}, N_{x,z}^\pm = \begin{bmatrix} B_x^\pm & A_x \\ A_x & FB_x^\pm \end{bmatrix}, A_w = \begin{bmatrix} w & -w \\ -w & w \end{bmatrix}, B_w^\pm = \begin{bmatrix} w & \pm 1 - w \\ \pm 1 - w & w \end{bmatrix},$$

$$F = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, w \in \{x, z\}, \text{ and } P \in 1 \oplus \mathcal{P}_3.$$

**Proof:** The ‘if’ part is obvious and easy to check. To prove the ‘only if’ part consider the following cases. First assume that the symbolic permutative orthogonal matrix $A$ has no
repetition of entries in any of the columns. Besides, since rows and columns are orthogonal, none of $P, Q, R$ are equal to each other. Then $A$ can presume one of the following forms:

$$X = \begin{bmatrix} x & y & z & w \\ y & x & w & z \\ z & w & y & x \\ w & z & x & y \end{bmatrix}, \quad Y = \begin{bmatrix} x & y & z & w \\ y & z & w & x \\ z & w & x & y \\ w & x & y & z \end{bmatrix}, \quad Z = \begin{bmatrix} x & y & z & w \\ y & w & x & z \\ z & x & w & y \\ w & y & z & x \end{bmatrix}$$

for some $x, y, z, w \in \mathbb{C}$.

Thus each of the four system of equations gives rise to the following sets of matrices obeying the pattern $X$:

$$\mathcal{X}_1 = \left\{ \begin{bmatrix} A_x & B^+ \\ B^+ & -A_x \end{bmatrix} : x^2 + z^2 - z = 0 \right\}, \quad \mathcal{X}_2 = \left\{ \begin{bmatrix} A_x & B^- \\ B^- & -A_x \end{bmatrix} : x^2 + z^2 + z = 0 \right\},$$

$$\mathcal{X}_3 = \left\{ \begin{bmatrix} B^+_x & A_x \\ A_x & FB^+_x \end{bmatrix} : x^2 + z^2 - x = 0 \right\}, \quad \mathcal{X}_4 = \left\{ \begin{bmatrix} B^-_x & A_x \\ A_x & FB^-_x \end{bmatrix} : x^2 + z^2 + x = 0 \right\}.$$  

Hence,

$$\mathcal{X}_1 = \{M^+_{x, z} : x^2 + z^2 - z = 0\}, \quad \mathcal{X}_2 = \{M^-_{x, z} : x^2 + z^2 + z = 0\},$$

$$\mathcal{X}_3 = \{N^+_{x, z} : x^2 + z^2 - x = 0\}, \quad \mathcal{X}_4 = \{N^-_{x, z} : x^2 + z^2 + x = 0\},$$

where $M^\pm_{x, z}, N^\pm_{x, z}, A_w, B_w, w \in \{x, z\}$ are defined in the statement of the theorem.

Similarly the orthogonality of the symbolic matrix $Y$ implies that $(x, y, z, w)$ must satisfy the system of polynomial equations

$$\begin{cases} x + y + z + w \in \{1, -1\} \\ xy + zw = 0 \Rightarrow x^2 + z^2 \mp z = 0 \quad \text{or} \quad y^2 + z^2 \mp x = 0 \quad \text{or} \quad x + y = 0 \quad \text{or} \quad z + w = 0 \\ x^2 + y^2 + z^2 + w^2 = 1 \quad \text{or} \quad z + w \mp 1 = 0 \quad \text{or} \quad x + y = 1 \quad \text{or} \quad x + y + z + w = \pm 1. \end{cases} \quad (3)$$

Thus each of the four system of equations gives rise to the following sets of matrices obeying the pattern $Y$:

$$\mathcal{Y}_1 = \left\{ P_{(23)} \begin{bmatrix} A_x & B^+_y \\ B^+_y & -A_x \end{bmatrix} P_{(23)} : x^2 + y^2 - y = 0 \right\}, \quad \mathcal{Y}_2 = \left\{ P_{(23)} \begin{bmatrix} A_x & B^-_y \\ B^-_y & -A_x \end{bmatrix} P_{(23)} : x^2 + y^2 + y = 0 \right\},$$

$$\mathcal{Y}_3 = \left\{ P_{(23)} \begin{bmatrix} B^+_x & A_y \\ A_y & FB^+_x \end{bmatrix} P_{(23)} : x^2 + y^2 - x = 0 \right\}, \quad \mathcal{Y}_4 = \left\{ P_{(23)} \begin{bmatrix} B^-_x & A_y \\ A_y & FB^-_x \end{bmatrix} P_{(23)} : x^2 + y^2 + x = 0 \right\}.$$  

Note that, $A = P_{(23)}M^+_{x, y}P_{(23)}$ if $A \in \mathcal{Y}_1$; $A = P_{(23)}M^-_{x, y}P_{(23)}$ if $A \in \mathcal{Y}_2$; $A = P_{(23)}N^+_{x, y}P_{(23)}$ if $A \in \mathcal{Y}_3$, and $A = P_{(23)}N^-_{x, y}P_{(23)}$ if $A \in \mathcal{Y}_4$ where $(x, y)$ satisfies the respective constraint as given in equation (6).

Finally the orthogonality of the symbolic matrix $Z$ implies that $(x, y, z, w)$ must satisfy the system of polynomial equations

$$\begin{cases} x + y + z + w \in \{1, -1\} \\ xy + wz = 0 \Rightarrow x^2 + y^2 \mp y = 0 \quad \text{or} \quad y^2 + x^2 \mp x = 0 \quad \text{or} \quad y + z = 0 \quad \text{or} \quad x + w = 0 \\ x^2 + y^2 + z^2 + w^2 = 1 \quad \text{or} \quad y + z \mp 1 = 0 \quad \text{or} \quad x + w = 1 \quad \text{or} \quad x + w + z + w = \pm 1. \end{cases} \quad (7)$$

4
Thus each of the four system of equations gives rise to the following set of matrices obeying the pattern $Z$:

$$Z_1 = \left\{ P_{(24)} \begin{bmatrix} A_x & B_y^+ \\ B_y & -A_x \end{bmatrix} P_{(24)} : x^2 + y^2 - y = 0 \right\}, \quad Z_2 = \left\{ P_{(24)} \begin{bmatrix} A_x & B_y^- \\ B_y & -A_x \end{bmatrix} P_{(24)} : x^2 + y^2 + y = 0 \right\},$$

$$Z_3 = \left\{ P_{(24)} \begin{bmatrix} B_y^+ & A_y \\ A_y & FB_x^2 \end{bmatrix} P_{(24)} : x^2 + y^2 - x = 0 \right\},$$

$$Z_4 = \left\{ P_{(24)} \begin{bmatrix} B_x & A_y \\ A_y & FB_x^2 \end{bmatrix} P_{(24)} : x^2 + y^2 + x = 0 \right\} \quad (8)$$

Besides, $A = P_{(24)}M_{x,y}^+P_{(24)}$ if $A \in Z_1$; $A = P_{(24)}M_{x,y}^-P_{(24)}$ if $A \in Z_2$; $A = P_{(24)}N_{x,y}^+P_{(24)}$ if $A \in Z_3$; and $A = P_{(24)}N_{x,y}^-P_{(24)}$ if $A \in Z_4$.

Next, consider the symbolic permutative orthogonal matrices $A$, in which one entry is repeated in at least one column i.e. the case when $P, Q, R$ are not chosen from any of the collection

$$\{P_{(12)(34)}, P_{(1324)}, P_{(1432)}, P_{(1423)}, P_{(1342)}, P_{(1234)}, P_{(1243)}\}.$$

Then it follows that $A$ belongs to either of the sets $X = \bigcup_{k=1}^4 X_k, Y = \bigcup_{k=1}^4 Y_k, Z = \bigcup_{k=1}^4 Z_k$ for certain values of $x, y, z$. In particular, a straightforward calculation shows that any symbolic permutative orthogonal matrix whose entries do not follow the pattern of entries of $X, Y, Z$ are $\pm P$ or $\pm (1/2J - P)$ for some $\tau \in S_4$. Then the desired result follows from the fact that permutation of the rows preserves the orthogonality and permutative property of a matrix.

Next remark follows from Theorem 2.1.

**Remark 2.2.** (Permutative orthogonal matrix as linear sum of permutations) Any permutative orthogonal matrix $A$ of order $4 \times 4$ can be written as linear sum of permutation matrices as follows:

$$P^T A = \begin{cases} xP_{(34)} + yP_{(12)} + zP_{(13)(24)} + wP_{(14)(23)}, & \text{when } A \in X \\ xP_{(24)} + yP_{(12)(34)} + zP_{(13)} + wP_{(14)(23)}, & \text{when } A \in Y \\ xP_{(23)} + yP_{(12)(34)} + zP_{(13)(24)} + wP_{(14)}, & \text{when } A \in Z \end{cases}$$

and $P \in 1 \oplus P_3$.

Let us emphasize that one of the motivations for the characterization of permutative orthogonal matrices is to use such a matrix as the coin operator for quantum walks on a 2 dimensional lattice. The standard coin operator of a coined quantum walk on 2 dimensional lattice is the Grover matrix of order $4 \times 4$ which is a permutative orthogonal matrix that enables the walker to explore four possible orthogonal directions to move on the lattice [10]. Indeed, the Grover coin of order $4 \times 4$ is given by

$$G = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \quad (10)$$

Then it can be seen that

$$G = \begin{cases} P_{(34)} \left( xP_{(34)} + yP_{(12)} + zP_{(13)(24)} + wP_{(14)(23)} \right) \in X \\ P_{(24)} \left( xP_{(24)} + yP_{(12)(34)} + zP_{(13)} + wP_{(14)(23)} \right) \in Y \\ P_{(23)} \left( xP_{(23)} + yP_{(12)(34)} + zP_{(13)(24)} + wP_{(14)} \right) \in Z \end{cases}$$

where $x = -\frac{1}{2}, y = \frac{1}{2} = z = w$. In particular, it follows that

$$G \in \text{Gro} = P_{(34)}X_1 \cup P_{(24)}Y_1 \cup P_{(23)}Z_1 \quad (11)$$
where

\[
X_1 = \begin{bmatrix}
  x & -x & z & 1 - z \\
  -x & x & 1 - z & z \\
  z & 1 - z & -x & x \\
  1 - z & z & x & -x \\
\end{bmatrix} : x^2 + z^2 - z = 0,
\]

\[
Y_1 = \begin{bmatrix}
  x & y & 1 - y & -x \\
  y & -x & 1 - y & x \\
  -x & 1 - y & y & x \\
  1 - y & x & y & -x \\
\end{bmatrix} : x^2 + y^2 - y = 0,
\]

\[
Z_1 = \begin{bmatrix}
  x & y & 1 - y & -x \\
  y & -x & 1 - y & x \\
  -x & 1 - y & y & x \\
  1 - y & x & y & -x \\
\end{bmatrix} : x^2 + y^2 - y = 0.
\]

Hence the sets of matrices \( P_{(34)}X_1, P_{(24)}Y_1, P_{(23)}Z_1 \) can be considered as the continuous families of orthogonal matrices that are generalizations of Grover matrix. We call the real orthogonal matrices in Grov as generalized Grover coins. In Section 3 we utilize these matrices as coin operators for quantum walks on two-dimensional lattices, and we investigate the localization property of the corresponding quantum walks.

In the following we determine certain chains of groups of permutative orthogonal matrices. It is computational to check that \( \det(A) = 1 \) if \( A \in \{ X_j, Y_j, Z_j : j = 1, 2 \} \), and \( \det(A) = -1 \) if \( A \in \{ X_j, Y_j, Z_j : j = 3, 4 \} \), where \( X_j, Y_j, Z_j, j = 1, 2, 3, 4 \) are given by equations (4), (6), (8) respectively.

**Theorem 2.3.** The following are chains of groups of complex orthogonal matrices.

1. \[ \{ I \} \leq P_{(34)}X_3 \leq P_{(34)}X_3 \cup P_{(34)}X_j \leq P_{(34)}X_3 \cup P_{(34)}X_j \cup X_3 \cup X_j \leq O_4, \]
   \[ \{ I \} \leq P_{(34)}X_3 \leq P_{(34)}X_3 \cup X_j \leq P_{(34)}X_3 \cup X_3 \cup X_j \leq O_4 \]

2. \[ \{ I \} \leq P_{(24)}Y_3 \leq P_{(24)}Y_3 \cup P_{(24)}Y_j \leq P_{(24)}Y_3 \cup P_{(24)}Y_j \cup Y_3 \cup Y_j \leq O_4, \]
   \[ \{ I \} \leq P_{(24)}Y_3 \leq P_{(24)}Y_3 \cup Y_j \leq P_{(24)}Y_3 \cup Y_3 \cup Y_j \leq O_4 \]

3. \[ \{ I \} \leq P_{(23)}Z_3 \leq P_{(23)}Z_3 \cup P_{(23)}Z_j \leq P_{(23)}Z_3 \cup P_{(23)}Z_j \cup Z_3 \cup Z_j \leq O_4, \]
   \[ \{ I \} \leq P_{(23)}Z_3 \leq P_{(23)}Z_3 \cup Z_j \leq P_{(23)}Z_3 \cup Z_3 \cup Z_j \leq O_4 \]

where \( j = 1, 2, 3, 4 \) and \( O_4 \) denotes the group of complex orthogonal matrices of order 4.

**Proof:** First we prove that \( P_{(34)}X_3 \cup P_{(34)}X_j \cup X_3 \cup X_j \) are complex orthogonal matrix groups for \( j = 1, 2, 3, 4 \). Clearly \( I \in P_{(34)}X_3 \cup P_{(34)}X_j \cup X_3 \cup X_j \). If \( A \in P_{(34)}X_3 \) then \( AT \in P_{(34)}X_3 \) follows from exchanging the role of \( z \) and \( -z \). Similarly, \( AT \in P_{(34)}X_j \) if \( A \in P_{(34)}X_j \) for \( j = 1, \ldots, 4 \). Since \( X_j \) and \( X_3 \) contain complex symmetric matrices, obviously \( A^T \in X_j \) if \( A \in X_j \), and \( A^T \in X_3 \) if \( A \in X_3 \). Hence, \( P_{(34)}X_3 \cup P_{(34)}X_j \cup X_3 \cup X_j \) is closed under inverses.

Let \( A = x_1 I + y_1 P_{(12)(34)} + z_1 P_{(1324)} + w_1 P_{(1423)} \), \( B = x_2 I + y_2 P_{(12)(34)} + z_2 P_{(1324)} + w_2 P_{(1423)} \) in \( P_{(34)}X_3 \cup P_{(34)}X_j \), \( j = 1, \ldots, 4 \), where \( (x_i, y_i, z_i, w_i), i = 1, 2 \) satisfy the equation given by (3). Then \( AB = x_3 I + y_3 P_{(12)(34)} + z_3 P_{(1324)} + w_3 P_{(1423)} \) where

\[
x_3 = x_1 x_2 + y_1 y_2 + z_1 w_2 + w_1 z_2,
\]

\[
y_3 = x_1 y_2 + y_1 x_2 + z_1 z_2 + w_1 w_2,
\]

\[
z_3 = x_1 z_2 + y_1 w_2 + z_1 x_2 + w_1 y_2,
\]

\[
w_3 = x_1 w_2 + y_1 z_2 + z_1 y_2 + w_1 x_2.
\]

Now, \( x_3 + y_3 + z_3 + w_3 = (x_1 + y_1 + z_1 + w_1)(x_2 + y_2 + z_2 + w_2) \) so that \( x_3 + y_3 + z_3 + w_3 = \)

\[
\begin{cases}
1 & \text{if } A, B \in P_{(34)}X_3 \cup P_{(34)}X_j \text{ or } P_{(34)}X_2 \cup P_{(34)}X_4 \\
-1, & \text{otherwise}.
\end{cases}
\]


Further
\[ x_3^2 + y_3^2 + z_3^2 + w_3^2 = \begin{bmatrix} x_1 \\ y_1 \\ z_1 \\ w_1 \end{bmatrix}^T \begin{bmatrix} a & b & c \\ b & a & c \\ c & c & a \\ c & c & b \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \\ z_1 \\ w_1 \end{bmatrix}, \]

where \( a = x_3^2 + y_3^2 + z_3^2 + w_3^2 = 1, b = 2x_2y_2 + 2z_2w_2 = 0 \) and \( c = (x_2 + y_2)(z_2 + w_2) = 0 \). This implies \( x_3^2 + y_3^2 + z_3^2 + w_3^2 = x_1^2 + y_1^2 + z_1^2 + w_1^2 = 1 \). Also,
\[
\begin{align*}
x_3 + y_3 &= (x_1 + y_1)(x_2 + y_2) + (z_1 + w_1)(z_2 + w_2) \\
z_3 + w_3 &= (x_1 + y_1)(z_2 + w_2) + (z_1 + w_1)(x_2 + y_2).
\end{align*}
\]

(12)

Hence \( AB \in \begin{cases} P_{(34)}X_3 & \text{if } A, B \in P_{(34)}X_j, \\ P_{(34)}X_j & \text{if either } A \text{ or } B \in P_{(34)}X_j, \end{cases} \)

for \( j = 1, \ldots, 4 \). Thus \( AB \in P_{(34)}X_3 \cup P_{(34)}X_j \) for \( j = 1, \ldots, 4 \).

Now let \( A = x_1P_{(34)} + y_1P_{(12)} + z_1P_{(13)(24)} + w_1P_{(14)(23)}, B = x_2P_{(34)} + y_2P_{(12)} + z_2P_{(13)(24)} + w_2P_{(14)(23)} \in X_3 \cup X_j \) where \( (x_i, y_i, z_i, w_i), i = 1, 2 \) satisfy the equations in (3) and \( j, k = 1, \ldots, 4 \). Then
\[
\begin{align*}
x_3 &= x_1x_2 + y_1y_2 + z_1z_2 + w_1w_2, \\
y_3 &= x_1y_2 + y_1x_2 + z_1w_2 + w_1z_2, \\
z_3 &= x_1z_2 + y_1w_2 + z_1y_2 + w_1x_2, \\
w_3 &= x_1w_2 + y_1z_2 + z_1x_2 + w_1y_2.
\end{align*}
\]

Hence
\[
x_3 + y_3 + z_3 + w_3 = \begin{cases} 1 & \text{if } A, B \in X_1 \cup X_3 \text{ or } X_2 \cup X_4, \\ -1, & \text{otherwise}. \end{cases}
\]

Then as above, \( x_3^2 + y_3^2 + z_3^2 + w_3^2 = 1 \). Further, \( x_3 + y_3 \) and \( z_3 + w_3 \) are same as (12). Hence
\[
AB \in \begin{cases} P_{(34)}X_3 & \text{if } A, B \in X_j, \\ P_{(34)}X_j & \text{if either } A \text{ or } B \in X_j, \end{cases} \)

for \( j = 1, \ldots, 4 \). Thus \( AB \in P_{(34)}X_3 \cup P_{(34)}X_j \) for \( j = 1, \ldots, 4 \).

Let \( A = x_1I + y_1P_{(12)(34)} + z_1P_{(13)(24)} + w_1P_{(14)(23)} \in P_{(34)}X_j \) and \( B = x_2P_{(34)} + y_2P_{(12)} + z_2P_{(13)(24)} + w_2P_{(14)(23)} \in \mathcal{X}_k \) for \( j, k = 1, \ldots, 4 \) and \( (x_i, y_i, z_i, w_i), i = 1, 2 \) are given by 3. Then \( AB = x_3P_{(34)} + y_3P_{(12)} + z_3P_{(13)(24)} + w_3P_{(14)(23)} \), where
\[
\begin{align*}
x_3 &= x_1x_2 + y_1y_2 + z_1z_2 + w_1w_2, \\
y_3 &= x_1y_2 + y_1x_2 + z_1w_2 + w_1z_2, \\
z_3 &= x_1z_2 + y_1w_2 + z_1y_2 + w_1x_2, \\
w_3 &= x_1w_2 + y_1z_2 + z_1x_2 + w_1y_2.
\end{align*}
\]

Thus
\[
x_3 + y_3 + z_3 + w_3 = \begin{cases} 1 & \text{if } A \in P_{(34)}X_1 \cup P_{(34)}X_3 \text{ and } B \in X_1 \cup X_3, \\ -1, & \text{otherwise}. \end{cases}
\]

It can be checked as above that \( x_3^2 + y_3^2 + z_3^2 + w_3^2 = 1 \). Further, \( x_3 + y_3 \) and \( z_3 + w_3 \) are given by (12).

Hence \( AB \in \begin{cases} \mathcal{X}_3 \text{ if } A = P_{(34)}X_j \text{ and } B \in X_j, j = 1, \ldots, 4, \\ \mathcal{X}_j \text{ if } A = P_{(34)}X_j \text{ and } B \in \mathcal{X}_k, j \neq k, (j, k) \in \{(1, 2), (3, 4)\}, \\ \mathcal{X}_1 \text{ if } A = P_{(34)}X_3 \text{ and } B \in \mathcal{X}_k, j \neq k, (j, k) \in \{(1, 3), (2, 4)\}, \\ \mathcal{X}_3 \text{ if } A = P_{(34)}X_3 \text{ and } B \in \mathcal{X}_k, j \neq k, (j, k) \in \{(1, 4), (2, 3)\}. \end{cases} \)

Thus all these yield that \( P_{(34)}X_3 \cup P_{(34)}X_j \cup P_{(34)}X_j \cup \mathcal{X}_3 \cup \mathcal{X}_j, j = 1, \ldots, 4 \) are groups with respect to matrix multiplication.

Let \( G \) represent any matrix group from the chain of groups corresponding to \( \mathcal{X}_j \). Now by Theorem 2.1 we observe that if \( D \in \mathcal{X}_k \) then there exist \( B \in \mathcal{Y}_k \) and \( C \in \mathcal{Z}_k \) such that \( B = P_{(23)}DP_{(23)} \) and \( C = P_{(24)}DP_{(24)} \), \( k = 1, \ldots, 4 \). Thus the chains corresponding to \( \mathcal{Y}_3 \) and \( \mathcal{Z}_3 \) follows from the observation that \( f : G \to G' \), is a group isomorphism defined by
f(X) = P(23)XP(23) and f(X) = P(24)XP(24) when G’ is the image of the map f. Note that
P(23)' = P(23), P(24)' = P(24).

Now we include some remarks about Proposition 2.3.

Remark 2.4. 1. P(34)\mathcal{X}_3, P(24)\mathcal{Y}_3 and P(23)\mathcal{Z}_3 are commutative matrix groups such that
any matrix A in these groups can be written as A = xI + yP + zP^2 + wP^3, where
P = P(342) if A \in P(34)\mathcal{X}_3, P = P(1234) if A \in P(24)\mathcal{Y}_3, and P = P(342) if A \in P(23)\mathcal{Z}_3.

2. It may be observed that \mathcal{PO}_4 is not closed under matrix multiplication and hence it does
not form a group. For instance, consider

\[ A = \begin{bmatrix} \frac{-2}{3} & -\frac{4}{3} & 1 \\ -\frac{2}{3} & \frac{4}{3} & \frac{-1}{3} \\ \frac{2}{3} & \frac{-4}{3} & \frac{-1}{3} \end{bmatrix} \in \mathcal{X}_1 \text{ and } B = \begin{bmatrix} \sqrt{2} & \frac{-2}{3} & \frac{-2}{3} \\ \frac{-4}{3} & \frac{2}{3} & \frac{-2}{3} \\ \frac{2}{3} & \frac{-2}{3} & \frac{-2}{3} \end{bmatrix} \in \mathcal{Y}_1, \]

then clearly AB = \[ \begin{bmatrix} \frac{-2\sqrt{2}}{3} & 1 & \frac{2\sqrt{2}}{3} \\ \frac{-2\sqrt{2}}{3} & 1 & \frac{2\sqrt{2}}{3} \\ \frac{-2\sqrt{2}}{3} & 1 & \frac{2\sqrt{2}}{3} \end{bmatrix} \notin \mathcal{PO}_4. \]

However, recall that the set of all 3 \times 3 permutative orthogonal matrices forms a matrix
group \([22]\).

Next we classify all permutative orthogonal matrices that are real.

Corollary 2.5. Any real permutative orthogonal matrix A \in \mathcal{X}_R \cup \mathcal{Y}_R \cup \mathcal{Z}_R where

\[ \mathcal{X}_R = \{ PM_{x,z}^s, PN_{z,x}^s : x, z \in \mathbb{R}, s = \pm \} \]

\[ \mathcal{Y}_R = \{ PP(23)M_{x,x}^s, PP(24)N_{x,x}^s : x, z \in \mathbb{R}, s = \pm \} \]

\[ \mathcal{Z}_R = \{ PP(34)M_{x,z}^s, PP(23)N_{x,z}^s : x, z \in \mathbb{R}, s = \pm \} \]

and

\[ M_{x,z}^s = \begin{bmatrix} A_x & B_z^s \\ B_x^s & -A_z \end{bmatrix}, N_{x,z}^s = \begin{bmatrix} B_x^s & A_z \\ A_x & FB_x^s \end{bmatrix}, A_w = \begin{bmatrix} w & -w \\ -w & w \end{bmatrix}, B_w^\pm = \begin{bmatrix} w & \pm 1-w \\ \pm 1-w & w \end{bmatrix}, F = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \]

x = \pm \sqrt{z(1-z)}, 0 \leq z \leq 1 \text{ if } s = +; \text{ and } x = \pm \sqrt{-z(1+z)}, -1 \leq z \leq 0 \text{ if } s = -;

P \in 1 \oplus P_3, w \in \{x, z\}.

Now we determine the set of permutative orthogonal matrices that are rational as follows.

Treating \(x^2 - x + z^2 = 0\) as a polynomial in indeterminate x, we obtain

\[ x = \frac{1 \pm \sqrt{1 - 4z^2}}{2}. \]

Then x \in \mathbb{Q} if and only if 1 - 4z^2 is zero or perfect square of a nonzero rational number of the
form p/q for p, q \in \mathbb{Z}, q \neq 0. It is zero if z \in \{-\frac{1}{2}, \frac{1}{2}\}. If 1 - 4z^2 = \frac{p^2}{q^2} \text{ for } p/q \neq 0 \text{ then after rewriting it takes the form } X^2 - 4Y^2 = 1, \text{ where } X = q/p \text{ and } Y = zq/p. \text{ Now } (X + 2Y) \text{ and}
(X - 2Y) \text{ are units in } \mathbb{Q} \text{ for } z \in \mathbb{Q} \text{ such that } (X + 2Y)(X - 2Y) = 1. \text{ Thus letting } X + 2Y = r
\text{ and } X - 2Y = \frac{1}{r} \text{ for some nonzero } r \in \mathbb{Q}, \text{ we obtain}

\[ X = \frac{1}{2} \left( r + \frac{1}{r} \right) \text{ and } Y = \frac{1}{4} \left( r - \frac{1}{r} \right). \]

Consequently we have the following corollary which describes set of all permutative orthogonal
matrices that are rational.
Corollary 2.6. Any rational permutative orthogonal matrix $A \in X_{Q} \cup Y_{Q} \cup Z_{Q}$ where

\[ X_{Q} = \{ PM_{x,z}^{s}, PN_{z,x}^{s} : x, z \in Q, s = \pm \} \]

\[ Y_{Q} = \{ PP_{(23)}M_{x,z}^{s}P_{(23)}, PP_{(23)}N_{x,z}^{s}P_{(23)} : x, z \in Q, s = \pm \} \]

\[ Z_{Q} = \{ PP_{(24)}M_{x,z}^{s}P_{(24)}, PP_{(24)}N_{x,z}^{s}P_{(24)} : x, z \in Q, s = \pm \} \]

and

\[ M_{x,z}^{s} = \begin{bmatrix} A_{x} & B_{x}^{s} \\ B_{z}^{s} & -A_{z} \end{bmatrix} \]

\[ N_{x,z}^{s} = \begin{bmatrix} B_{x}^{s} & A_{z} \\ A_{z} & FB_{z}^{s} \end{bmatrix} \]

\[ A_{w} = \begin{bmatrix} w & -w \\ -w & w \end{bmatrix}, B_{w}^{\pm} = \begin{bmatrix} w & \pm 1 - w \\ \pm 1 - w & w \end{bmatrix}, F = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \]

\[ x = \frac{r^2 - 1}{2(r^2 + 1)}, \quad z = \frac{1}{2} + \frac{r}{r^2 + 1}, \quad \text{if } s = +; \quad \text{and } x = \frac{r^2 - 1}{2(r^2 + 1)}, \quad z = -\frac{1}{2} + \frac{r}{r^2 + 1}, \quad \text{if } s = -; \]

\[ P \in 1 \oplus \mathcal{P}_{3}, w \in \{ x, z \}. \]

It is also not hard to check that the chains of matrix groups described in Proposition 2.3 remains valid when the subgroups are restricted only for the real or rational matrices as given in Corollary 2.5 and Corollary 2.6.

2.1 Search for orthogonal matrices that are linear sum of permutation matrices but not permutative

In [22], it is shown that an orthogonal matrix of order $3 \times 3$ is a linear sum of permutations if and only if it is permutative. However, this is no longer true for $4 \times 4$ matrices. For instance, consider the orthogonal matrix

\[ A = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{2}J_{3} - J_{3}^{2} \end{bmatrix} = -\frac{1}{2}I + \frac{2}{3}P_{(234)} + \frac{2}{3}P_{(243)}, \]

which is a linear sum of permutations but not permutative, where $J_{3}$ is the all-one matrix of order $3 \times 3$. Indeed, it may be noted that this matrix $A$ is a direct sum of two permutative matrices. Then the following question arises: Does there exist any orthogonal matrix of order $4 \times 4$ that is a linear sum of permutations but neither a permutative matrix nor a direct sum of permutative matrices up to permutations of its rows and columns? In this section we carry out search for such matrices. Indeed, answer to this question has implications for the characterization of all orthogonal matrices that are linear sum of permutations, which remained an open problem in literature.

First we derive certain sufficient conditions for which an orthogonal matrix which is a linear sum of permutation matrices is always permutative, that is, such a matrix can always be written in the form given by equation (9). Besides, recall that a necessary condition for a linear sum of permutation matrices to be real orthogonal is that sum of the entries along a row or column should be $\pm 1$ [12]. We provide an alternative easy proof of this result for complex orthogonal matrices of order $4 \times 4$ in the following proposition.

Proposition 2.7. A necessary condition for a linear sum of permutation matrices $A$ of order $4 \times 4$ to be orthogonal is that the sum of the entries along each row and column is $\pm 1$.

Proof: Let $A = \sum_{\sigma \in S_{n}} x_{\sigma}P_{\sigma}$, where $P_{\sigma} \in \mathcal{P}_{4}$ the permutation matrix corresponding to the permutation $\sigma \in S_{4}$, the permutation group of order 4. The $i^{th}$ row sum of $A$ is

\[ A_{(i,:)} = \sum_{j=1}^{4} \sum_{\sigma} x_{\sigma}P_{\sigma}(i, j) = \sum_{\sigma} x_{\sigma} \sum_{j=1}^{n} P_{\sigma}(i, j) = \sum_{\sigma} x_{\sigma}. \]

Similarly, each column sum of $A$ is $\sum_{\sigma} x_{\sigma}$. Then consider the Hardamard matrix of order $4 \times 4$ as follows:

\[ H = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}. \]
\[ B = H^T AH = \begin{bmatrix} \sum x_\sigma & 0 \\ 0^T & \bar{A} \end{bmatrix}, \]

where \( \mathbf{0} \in \mathbb{R}^3 \) is the zero vector and \( \bar{A} \) is a 3 × 3 orthogonal matrix. Then \( \sum x_\sigma \in \{\pm 1\} \) since B is orthogonal.

We call a set of matrices \( S = \{A_1, A_2, \ldots, A_n\} \) pairwise H-orthogonal if Hadamard product of any pair of matrices \( A_i, A_j, i \neq j \), denoted by \( A_i \odot A_j \) is the zero matrix \( \mathbf{0} \), \( 1 \leq i, j \leq n \).

We denote \( \langle S \rangle = \{ \sum_{j=1}^n \alpha_j A_j : \alpha_j \in \mathbb{R} \} \) as the vector space generated by elements of \( S \).

Observe that any \( A \in \langle S \rangle \) is always permutative.

Then we have the following proposition.

**Proposition 2.8.** Any linear sum of permutation matrices of order 4 × 4 can be written as a sum of at most 6 permutative matrices each of which is a linear sum of 4 permutation matrices that are pairwise H-orthogonal.

**Proof:** The proof follows from the fact that the permutation group \( S_4 \) can be partitioned into disjoint collection of six permutations that correspond to H-orthogonal subsets described as follows:

\[
\{id, (12)(34), (13)(24), (14)(23)\}, \{(23), (124), (134), (143)\}, \\
\{(34), (12), (1234), (1423)\}, \{(14), (1243), (132), (234)\}, \\
\{(13), (1234), (142), (243)\}.
\]

This completes the proof.

Then we have the following theorem.

**Theorem 2.9.** Let \( A \in \langle S \rangle \) where \( S \) is pairwise H-orthogonal set that contains permutation matrices of order 4 × 4. Then any orthogonal matrix \( B \) of the form \( A + cP \) where \( P \in \mathcal{P}_4 \), is a permutative orthogonal matrix.

**Proof:** Obviously \( B = A \in \langle S \rangle \) is permutative if \( c = 0 \). Let \( c \neq 0 \). Let \( A \) be a symbolic permutative matrix with first row \( x = (x, y, z, w) \). Consider the entries \( A_{ij} \) for which \( P_{ij} = 1 \). Then \( B_{ij} = A_{ij} + c \) if and only if \( P_{ij} = 1 \); and \( B_{ij} = A_{ij} \) otherwise. For any pair of indices \( (i, j) \) and \( (k, l) \) with \( P_{ij} = 1 = P_{kl} \), the unit norm condition of rows of \( B \) implies \( A_{ij} = A_{kl} \) since \( c \neq 0 \). Obviously the permutative structure of \( A \) implies that \( B \) is permutative.

Below we show that no orthogonal matrix of order 4 can be a linear sum of two distinct permutation matrices. By non-trivial linear sum we mean all the coefficients of the linear sum are non-zero.

**Theorem 2.10.** There is no orthogonal matrix which is a non-trivial linear sum of two distinct permutation matrices.

**Proof:** Let \( A = \alpha P + \beta Q \) be an orthogonal matrix and \( P \neq Q \). If \( P \odot Q = 0 \) then \( A \) is a permutative orthogonal matrix. From the classification of all permutative matrices described in Theorem 2.1 it can be observed that any permutative orthogonal matrix is a linear sum of four H-orthogonal permutation matrices. Indeed, it follows from equations (3), (5), (7) that if one or more coefficients in the linear combination of H-orthogonal permutation matrices is zero, then the corresponding permutative orthogonal matrix becomes \( \pm M \) for some \( M \in \mathcal{P}_4 \).

Hence the desired result follows.

Next, assume that \( P \odot Q \neq 0 \). This means there can exist at most two pairs of indices \( (i, j) \) such that \( P_{ij} = Q_{ij} = 1 \) since \( P \neq Q \). Then \( A_{ij} = \alpha + \beta \) for those \( (i, j) \), and two permutation matrices \( X, Y \) can be found for which \( XAY = (\alpha + \beta)I_1 \oplus A_1 \) or \( (\alpha + \beta)I_2 \oplus A_2 \) where \( A_1 \) and \( A_2 \) are permutative orthogonal matrices of order 3 × 3 and 2 × 2 respectively. Indeed, each row of \( A_1 \) is a permutation of \( \{0, \alpha, \beta\} \); whereas each row of \( A_2 \) is a permutation of \( \{\alpha, \beta\} \). Then from the classification of permutative orthogonal matrices of order 3 × 3 (see Theorem 3.1, [22]) it can be seen that either \( (\alpha, \beta) = (\pm 1, 0) \) or \( (\alpha, \beta) = (0, \pm 1) \). The same holds for \( A_2 \), and hence the desired result follows.
The following theorem provides characterization of orthogonal matrices that are linear sum of three permutation matrices.

**Theorem 2.11.** If an orthogonal matrix \( A \) is a linear sum of three distinct permutation matrices then either \( A \) is a permutation matrix or \( XAY \) is a direct sum of permutative orthogonal matrices of order 3 and 1, for some permutation matrices \( X, Y \).

**Proof:** Let \( A = \alpha P + \beta Q + \gamma R \) be an orthogonal matrix which is a linear sum of permutation matrices \( P, Q, R \) of order \( 4 \times 4 \). Then two cases arise. Either the set \( S = \{ P, Q, R \} \) is pairwise \( H \)-orthogonal of there exist at least one pair of matrices in \( S \) whose Hadamard product is a non-zero matrix. Note that sum of entries of each row and column sums of \( A \) is \( \alpha + \beta + \gamma \).

First suppose that \( S \) is a pairwise \( H \)-orthogonal set then proceeding a similar argument as Proposition 2.10 it can be concluded that \( A = \pm M \) for some \( M \in \mathcal{P}_4 \). Next assume that \( S \) is not pairwise \( H \)-orthogonal. If there is only one pair of elements of \( S \) that are not \( H \)-orthogonal. Without loss of generality, let \( P \circ Q \neq 0 \). Then \( A_{ij} = \alpha + \beta \) if and only if \( P_{ij} = Q_{ij} = 1 \) for at most two indices \((i, j)\). Hence the orthonormality of \( A \) yields the polynomial system:

\[
\alpha^2 + \beta^2 + \gamma^2 = 1, \quad (\alpha + \beta)^2 + \gamma^2 = 1.
\]

Then it is computational to check that \( \alpha = 0 \) or \( \beta = 0 \). Then from Proposition 2.10 it follows that \( A = \pm M \) for some \( M \in \mathcal{P}_4 \). Now assume that there are two distinct pairs of matrices in \( S \) each of which are not \( H \)-orthogonal. Without loss of generality, let \( P \circ Q \neq 0, P \circ R \neq 0 \). Then \( A_{ij} = \alpha + \beta \) and \( A_{kl} = \alpha + \gamma \) if and only if \( P_{ij} = Q_{ij} = 1, P_{kl} = R_{kl} = 1 \) for some indices \((i, j)\) and \((k, l)\). Thus \((\alpha, \beta, \gamma)\) satisfy the following polynomial system due to the unit norm condition of rows of \( A \):

\[
(\alpha + \beta)^2 + \gamma^2 = 1, \quad (\alpha + \gamma)^2 + \beta^2 = 1.
\]

Solving these equations we have either \( \alpha = 0 \) or \( \beta = 0 \). If \( \alpha = 0 \), \( A \) is linear sum of \( Q \) and \( R \) and hence the desired result follows from Proposition 2.10, while for \( \beta = \gamma \) rows of \( A \) are permutations of \( x_1 = (\alpha + \beta, \beta, 0, 0) \) or \( x_2 = (\alpha, \beta, \beta, 0) \). If rows of \( A \) are permutations of \( x_1 \) only then \( \beta(\alpha + \beta) = 0 \). Otherwise if permutations of both \( x_1 \) and \( x_2 \) present as rows of \( A \) we obtain \( \alpha \beta = 0 \). Thus the result follows from Proposition 2.10. Finally, let all pairs of matrices from \( S \) are not \( H \)-orthogonal. Then if \( P \circ Q \circ R \neq 0 \) then there is exactly one index \((i, j)\) such that \( A_{ij} = \alpha + \beta + \gamma \) and \( P_{ij} = Q_{ij} = R_{ij} = 1 \) since \( P \neq Q \neq R \), which further implies that \( \alpha + \beta + \gamma \in \{\pm 1\} \). Obviously, two permutation matrices \( X, Y \) can be found such that \( XAY = (\alpha + \beta + \gamma) \oplus A_1 \) where \( A_1 \) is an \( 3 \times 3 \) orthogonal matrix which is linear sum of 3 permutation matrices. Then using the characterization of orthogonal matrices that are linear sum of permutations (see Theorem 3.2,[22]) we conclude that \( A_1 \) is a permutative orthogonal matrix and the desired result follows. Otherwise, if \( P \circ Q \neq 0, Q \circ R \neq 0, R \circ P \neq 0 \) with \( P \circ Q \circ R = 0 \) then each rows of \( A \) can be permutations of \((\alpha + \beta, \gamma, 0, 0)\), \((\alpha + \gamma, \beta, 0, 0)\) and \((\alpha, \beta + \gamma, 0, 0)\). However, all of these row vectors can not appear as rows of \( A \) simultaneously since column sum of \( A \) is \( \alpha + \beta + \gamma \) for each column. These complete the proof. \( \square \)

Now we focus on finding orthogonal matrices that are real linear sum of permutations but neither permutative nor a direct sum of permutative matrices up to permutations of rows or columns. Thus we investigate existence of such matrices belonging to subspaces generated by specific permutation matrices. Recall that the space of linear sum of permutation matrices of order \( n \) form a vector space, denoted by \( L \) over the field of real numbers of dimension \((n - 1)^2 + 1 \) [8]. For \( n = 4 \), we choose a basis \( B \) of \( L \) that contains 10 permutations given by:

\[
B = \{(12), (23), (24), (34), (123), (124), (234), (12)(34), (13)(24), (14)(23)\}.
\]

Let \( A \in L \). Then following the above arguments we write \( A \in \bigoplus_{k=1}^{5} L_k \) where \( L_k = \langle B_k \rangle \), \( k = 1, \ldots, 5 \) are subspaces of \( L \), generated by pairwise \( H \)-orthogonal sets of permutation matrices defined as follows:

\[
B_1 = \{P_{(12)}, P_{(34)}, P_{(13)(24)}, P_{(14)(23)}\}, B_2 = \{P_{(24)}, P_{(12)(34)}\},
\]

\[
B_3 = \{P_{(12)(34)}, P_{(234)}\}, B_4 = \{P_{(123)}\}, B_5 = \{P_{(23)}\}.
\]
If $A \in L_i, i = 1, \ldots, 5$, is orthogonal then $A$ can be characterized by Theorem 2.1 and hence $A \in \mathcal{PO}_4$.

Now we briefly review the concept of combinatorially orthogonal matrices introduced by Brualdi et al. [3] that will be used in sequel. A matrix having entries from \{0, 1\} is called a (0, 1) matrix. A nonzero pattern of a matrix $A$ is described by a (0, 1) matrix $B$ such that $b_{ij} = 1$ if and only if $a_{ij} \neq 0$ and $b_{ij} = 0$ otherwise. A pattern $M$ is orthogonal if there exists an (real) orthogonal matrix with the same pattern. Let $A$ be a (0, 1) matrix of order $n$. Then $A$ is combinatorially orthogonal or quadrangular if inner product of distinct rows or columns is not equal to 1. Let $S$ be a subset of rows of $A$ such that for each element of $S$ there is another element of $S$ with nonzero inner product. Then $A$ is said to be row strongly quadrangular if the matrix, whose rows are all the elements of $S$, has at least $|S|$ number of columns with at least two 1’s. Similarly, the matrix $A$ is said to be column strongly quadrangular if the set $S$ contains columns of $A$ and if the matrix whose columns are all the elements of $S$, has at least $|S|$ number of rows with at least two 1’s. If a (0, 1) matrix is both row and column strongly quadrangular then it is called strongly quadrangular.

Note that if a (0, 1) matrix supports unitary then it is strongly quadrangular but the converse need not be true. Now we recall the following proposition from [24].

**Proposition 2.12.** A (0, 1) matrix of degree $n \leq 4$ supports a unitary if and only if it is strongly quadrangular.

Then we have the following theorem.

**Theorem 2.13.** Let $A \in L_i \oplus L_j, i, j = 1, \ldots, 5$ be an orthogonal matrix. Then $A \in \mathcal{PO}_4$.

**Proof:** It is clear from Proposition 2.9 and Theorem 2.1 that $A \in \mathcal{PO}_4$ whenever $A \in L_i \oplus L_j$ for $i \neq j, i \in \{1, \ldots, 5\}, j \in \{4, 5\}$.

At first let $A = a_1P_{(12)} + a_2P_{(34)} + a_3P_{(13)(24)} + a_4P_{(14)(23)} + b_1P_{(24)} + b_2P_{(12)(34)} \in L_1 \oplus L_2$. The unit norm condition for rows of $A$ yield that at least one from each of the following is true \{b_2 = 0, a_1 = a_2\}, \{b_1 = 0, a_2 = a_3\} and \{b_1 = 0, a_1 = a_3\}. If $b_1 = b_2 = 0$, then $A \in L_1$. Otherwise while $b_1 \neq 0, b_2 = 0, a_1 = a_2 = a_3$, $A = A(x; P_{(1432)}, P_{(13)(24)}, P_{(12)(34)})$, where $x = (a_1 + b_1, a_1, a_1, a_3)$. When $b_1 = 0, b_2 \neq 0, a_2 = a_1$, then $A = A(x; P_{(12)(34)}, P_{(13)(24)}, P_{(14)(23)})$, where $x = (a_1, b_1 + a_2, a_3, a_4)$. At last for $b_1, b_2 \neq 0, a_2 = a_1$, $A = A(x; P_{(1432)}, P_{(13)(24)}, P_{(12)(34)})$, where $x = (a_1 + b_1, a_1 + b_2, a_1, a_4)$. Thus by Theorem 2.1 in all the above cases $A \in \mathcal{PO}_4$. If $A \in L_1 \oplus L_3$ then as above $A$ is linear sum of at most 6 permutations thus a similar arguments can be followed to show that $A \in \mathcal{PO}_4$

Secondly, suppose $A = b_1P_{(24)} + b_2P_{(12)(34)} + c_1P_{(124)} + c_2P_{(234)} \in L_2 \oplus L_3$. Then the (0, 1) pattern $M_A$ of $A$ is given by

$$M_A = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix},$$

which is not quadrangular. Hence $A$ is not an orthogonal matrix assuming that each entry of $A$ is nonzero. Let $M_i$ denote the $i$th column of $M$. Since $M_1^T M_4 = 1$ and $M_2^T M_3 = 1$ at least one holds from each of the two collections \{b_2 = 0, b_1 + c_1 = 0\} and \{b_2 = 0, b_1 + c_2 = 0\}. If $b_2 = 0$, then by Proposition 2.12 the nonzero pattern of $A$ can support an orthogonal matrix. Further unit norm of rows leads to either $b_1 = 0$ or $c_1 = c_2$. Whenever $b_2 = 0$ and $b_1 = 0$, $A \in L_3$. Otherwise for $c_1 = c_2$ together with $b_2 = 0$, $A$ reduces to a permutative matrix with two nonzero component in each row. Hence from Proposition 2.10, $A = \pm R, R \in \mathcal{P}_4$. If $b_2 \neq 0$ i.e. $b_1 + c_1 = 0$ and $b_1 + c_2 = 0$, a further analysis yields $c_1 = 0$. Hence $A = b_2P_{(12)(34)}$, where $b_2 = \pm 1$. These complete the proof. \qed

**Theorem 2.14.** Let $A \in L_i \oplus L_i \oplus L_j$ be orthogonal where $i, j \in \{2, 3, 4, 5\}$ and $(i, j) \notin \{(2, 5), (3, 4)\}$. Then $A \in \mathcal{PO}_4$.  

12
Proof: Since \( L_1 \) is generated by 4 \( H \)-orthogonal matrices whereas each of \( L_i \) and \( L_j \) are made up of one or two, the nonzero pattern of \( A \) is all 1 matrix in general. Let

\[
A = a_1P_{(12)} + a_2P_{(34)} + a_3P_{(13)(24)} + a_4P_{(14)(23)} + b_1P_{(24)} + b_2P_{(12)(34)} + c_1P_{(14)} + c_2P_{(12)(34)} + eP_{(23)} \in L_1 \oplus L_2 \oplus L_3.
\]

Then the unit norm condition of rows and columns of \( A \) yield the set of linear equations

\[
\begin{align*}
\{c_1 = 0, a_4 = a_1 + b_2, a_4 = a_2 + b_2, b_1 + c_1 = 0, a_3 = a_2\} \\
\{c_1 = 0, a_4 = a_2 + b_2, b_1 + c_1 = 0, a_3 = a_2\}.
\end{align*}
\]

Thus it can be verified that

1. If \( c_1 = c_2 = 0 \), then \( A \in L_1 \oplus L_2 \).

2. Consider \( c_1 = 0, c_2 \neq 0, a_4 = a_2 + b_2, b_1 + c_1 = 0, a_3 = a_2 \). Further \( A \) satisfies at least one condition from each of the collections \( \{b_2 = 0, a_1 = a_2\} \) and \( \{c_2 = 0, a_2 = a_4\} \).

3. If \( c_1 = 0, c_2 \neq 0, a_4 = a_2 + b_2, b_1 + c_2 = 0, a_3 = a_1 \), then we get either \( b_2 = 0 \) or \( a_1 = a_2 \).

Further it can be verified that in both the cases \( A \) cannot be orthogonal matrices under all the given conditions.

4. When \( c_1 = 0, c_2 \neq 0, a_4 = a_2 + b_2, a_3 = a_2 = a_1 \), then the orthonormality of \( A \) further implies \( a_4 = a_1 + b_1 \) and hence \( b_1 = b_2 \). So that \( A \) becomes \( A(x; P_{(1324)}, P_{(1423)}, P_{(12)(34)}) \) with \( x = (a_1 + c_2, a_4, a_1, a_4) \). A similar analysis can be done for all the cases where \( c_2 = 0 \) and \( c_1 \neq 0 \).

5. If \( c_1 \neq 0, c_2 \neq 0, a_4 = a_1 + b_2, a_1 = a_2, b_1 + c_1 = 0, b_1 + c_2 = 0 \), then \( A(x; P_{(1234)}, P_{(13)(24)}, P_{(1423)}) \) with \( x = (a_1, a_4 + c_1, a_3, a_4) \).

6. Consider \( c_1 \neq 0, c_2 \neq 0, a_1 = a_1 + b_2, a_4 = a_2 + a_3, b_1 + c_1 = 0 \). So that the orthogonality of \( A \) yields either \( a_1 = 0 \) or \( 2a_4 + c_2 = 0 \). For \( a_1 = 0 \) we get either \( a_4 = 0 \), hence \( A \in L_2 \oplus L_3 \) or \( b_1 + c_2 = 0 \), which goes with the previous case. Otherwise for \( 2a_4 + c_2 = 0 \) we get either \( b_1 = 2a_4 \), which is equivalent to say \( b_1 + c_2 = 0 \), or \( b_1 = 0 \), hence follows from Proposition 2.7 that \( A = \pm(1/2J - P_{(234)}) \). Similarly it can be done for \( c_1 \neq 0, c_2 \neq 0, a_4 = a_1 + b_2, a_1 = a_2 = a_3, b_1 + c_2 = 0 \).

7. If \( c_1 \neq 0, c_2 \neq 0, a_4 = a_1 + b_2, a_1 = a_3 = a_3 \), then the orthonormality of \( A \) yields either \( c_1 = c_2 \) or \( a_1 + b_1 = a_4 \). Now, \( c_1 = c_2 \) implies \( A = A(x; P_{(14)(23)}, P_{(13)(24)}, P_{(12)(34)}) \) with \( x = (a_1 + b_1 + c_1, a_4 + c_1, a_1, a_4) \). In particular \( A = \pm(1/2J - P) \), \( P \in \mathcal{P}_4 \). Whereas for \( a_1 + b_1 = a_4 \) we have \( b_1 = b_2 \) and \( A \) takes the form \( A(x; P_{(1324)}, P_{(1423)}, P_{(12)(34)}) \) with \( x = (a_4 + c_2, a_4 + c_1, a_1, a_4) \).

Using similar arguments of step by step elimination of entries of the polynomial system defined by orthonormality condition of the columns and rows of concerned matrices it can be verified that any orthogonal matrix belonging to a subspace from the following collection

\[
\{L_1 \oplus L_2 \oplus L_4, L_1 \oplus L_3 \oplus L_5, L_1 \oplus L_4 \oplus L_5\}
\]

is in \( \mathcal{PO}_4 \). \( \square \)

Theorem 2.15. Let \( A \in L_i \oplus L_j \oplus L_k \) be orthogonal where \( i, j, k \in \{2, 3, 4, 5\} \), then \( A \in \mathcal{PO}_4 \).

Proof: Clearly for all the given choices of \( i, j, k \), \( A \) can be the linear sum of at most 5 permutation matrices and non zero patterns of \( A \) are other than the all 1 matrix. Suppose, \( A = b_1P_{(24)} + b_2P_{(12)(34)} + c_1P_{(14)(23)} + c_2P_{(12)(34)} + eP_{(23)} \in L_2 \oplus L_3 \oplus L_5 \). Clearly the \((0, 1)\) pattern of \( A \) is not quadrangular and one from each of the collections \( \{b_2 = 0, b_1 + c_2 + e = 0\} \) and \( \{e = 0, b_2 + c_1 = 0\} \) is satisfied. Hence if \( e = 0 \) then \( A \in L_2 \oplus L_3 \). Otherwise if \( e \neq 0 \) and \( b_2 = 0 \) then \( c_1 = 0 \), so that nonzero pattern of \( A \),

\[
M_A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 \end{bmatrix}
\]
is non-quadrangular. A further analysis shows that $b_1$ should be 0 for $A$ to be orthogonal. Thus $A \in L_3 \oplus L_5$. Finally for $b_1 + c_2 + e = 0$ and $b_2 + c_1 = 0$ cannot hold simultaneously since $b_1 + b_2 + c_1 + c_2 + e \in \{ \pm 1 \}$ is a necessary condition for $A$ to be orthogonal. Hence the proof follows from Theorem 2.13.

Similarly by looking into the nonzero patterns and eliminating some entries for the requirement of orthogonality of $A$ we can prove for $A \in \{ L_2 \oplus L_3 \oplus L_4, L_2 \oplus L_4 \oplus L_5, L_3 \oplus L_4 \oplus L_5 \}$. □

**Theorem 2.16.** Let $A \in L_2 \oplus L_3 \oplus L_4 \oplus L_5$ be orthogonal. Then $A \in \mathcal{P}O_4$.

**Proof:** Let $A = b_1 P_{(24)} + b_2 P_{(12)(34)} + c_1 P_{(124)} + c_2 P_{(234)} + d P_{(123)} + e(23) \in L_2 \oplus L_3 \oplus L_4 \oplus L_5$. Let $M^k_A$ for $k = 1, \ldots, 4$ denote the $(0, 1)$ pattern of $A$ arise at different stages. Now,

$$M^1_A = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix},$$

which is not quadrangular. Since $R_i R^T_i = 1$ where $R_i$ denotes the $i^{th}$ row of $M^1_A$, either $b_2 = 0$ or $b_1 + c_2 + e = 0$ holds.

Hence if $b_2 = 0$, then

$$M^2_A = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 \end{bmatrix},$$

which is again not quadrangular since $C_i^T C_3 = 1 = C_2^T C_3$, where $C_i$ denotes the $i^{th}$ column of $M^2_A$. Thus at least one holds from each of the two collections $\{ d = 0, b_1 + c_1 = 0 \}$ and $\{ e = 0, b_1 + c_1 = 0 \}$. If $d = e = 0$, then $A \in L_2 \oplus L_3$. If $d = 0, e \neq 0$ then $A \in L_2 \oplus L_3 \oplus L_5$. Otherwise if $d \neq 0, e = 0$ then $A \in L_2 \oplus L_3 \oplus L_4$. Finally if $d \neq 0, e \neq 0, b_1 + c_1 = 0$. Then

$$M^3_A = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 \end{bmatrix},$$

and the orthogonality condition of $A$ implies either $d = 0$ or $e = 0$, which is a contradiction. Hence at least one of $d = 0$ or $e = 0$ holds whenever $b_2 = 0$.

If $b_2 \neq 0$ then $b_1 + c_2 + e = 0$ holds. Thus we get

$$M^4_A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix},$$

which is not quadrangular. Hence $\{ e = 0, b_2 + c_2 + d = 0 \}$ and $\{ (b_1 + c_2 = 0, b_2 + c_1 + d = 0 \}$ hold consecutively. So that $A \in L_2 \oplus L_3 \oplus L_4$ if $e = 0$. While for $e \neq 0$ we get $b_2 + c_1 + d = 0$ and thus $b_1 + b_2 + c_1 + c_2 + d = 0$. Which leads to a contradiction by Proposition 2.7. Thus the proof follows from Theorem 2.13 and Theorem 2.15. □

In all the cases above we determine spaces generated by specific permutation matrices such that any orthogonal matrix belonging to these spaces are either permutative or direct sum of permutative matrices after pre and post multiplication by permutation matrices to the original matrix. In the following we determine spaces of matrices such that this is no longer true. Indeed, we identify classes of orthogonal matrices belonging to certain spaces that are neither permutative nor direct sum of permutative matrices as follows.
Theorem 2.17. Let $A \in L_1 \oplus L_3 \oplus L_4$ be orthogonal. Then either $A \in \mathcal{PO}_4$ or there exists $P, Q \in \mathcal{P}_4$ such that $PAQ$ or $H(PAQ)H$ for some matrix $H$ is the Hadamard matrix and $\mathcal{PO}_3$ is the permutative orthogonal matrix group of order 3.

Proof: Suppose $A = a_1P(12) + a_2P(34) + a_3P(13)(24) + a_4P(14)(23) + c_1P(124) + c_2P(234) + dP(123) \in L_1 \oplus L_3 \oplus L_4$. Then the unit norm condition of rows and columns of $A$ yield the set of linear equations $\{c_2 = 0, a_2 = a_3\}, \{c_1 = 0, a_1 = a_3\}$ and $\{c_1 = 0, a_1 = a_4\}$ consecutively. Thus if $c_1 \neq 0$ and $c_2 \neq 0$ then we get $a_1 = a_2 = a_3 = a_4$ and a further computation shows that $d = 0$, which indicates $A \in L_1 \oplus L_3$. If $c_1 = c_2 = 0$, then $A \in L_1 \oplus L_4$. If $c_1 = 0, a_2 = a_3$ while $c_2 \neq 0$ then a further orthogonality conditions lead to either $a_1 = a_2$ or $d = 0$. If $d = 0$ then we are done. Suppose $a_1 = a_2$, with $c_1 = 0, a_2 = a_3$, so that $a_1 = a_2 = a_3$. Then the unit norm condition of rows of $A$ implies $a_1 = 0$ or $a_1 + a_4 + c_2 + d = 0$.

1. Now while $a_1 = 0$, we obtain

$$P(12)AP(13) = \begin{bmatrix} a_4 + c_2 + d & 0 & 0 & 0 \\ 0 & c_2 & d & a_4 \\ 0 & d & a_4 & c_2 \\ 0 & a_4 & c_2 & d \end{bmatrix},$$

and hence $a_4 + c_2 + d = \pm 1$.

2. For $a_1 + a_4 + c_2 + d = 0$ using Proposition 2.7 we obtain $3a_1 + a_4 + c_2 + d = \pm 1$ so that $a_4 + c_2 + d = a_1 \pm 1$. Hence when row sum of $A$ is 1 and $-1$, we obtain $a_1 = \frac{1}{2}$ and $a_1 = -\frac{1}{2}$ respectively. Hence $P(12)AP(13)$ belongs to one of the following sets.

$$\mathcal{C}_1 = \begin{cases} \begin{bmatrix} -\frac{1}{4} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} : a_4 = -\frac{1}{2}c_2 \pm \frac{1}{2}\sqrt{(1-3c_2)(1+c_2)}, -1 \leq c_2 \leq \frac{1}{3} \end{cases} \text{ and}$$

$$\mathcal{C}_2 = \begin{cases} \begin{bmatrix} -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} \end{bmatrix} : a_4 = -\frac{1}{2}c_2 \pm \frac{1}{2}\sqrt{(1+3c_2)(1-c_2)}, -\frac{1}{3} \leq c_2 \leq 1 \end{cases}.$$  

Then observe that $HMH = \begin{bmatrix} 1 & 0 \\ 0 & M_1 \end{bmatrix}$ if $M \in \mathcal{C}_1$ for some matrix $M_1 \in \mathcal{C}_1$, and $HNH = \begin{bmatrix} 1 & 0 \\ 0 & N_2 \end{bmatrix}$ if $N \in \mathcal{C}_2$ for some matrix $N_2 \in \mathcal{C}_2$, where

$$\mathcal{C}_1 = \begin{cases} \begin{bmatrix} -\frac{1}{2} & a_4 \\ -\frac{1}{2} & -a_4 - c_2 \\ c_2 & -\frac{1}{2} + a_4 \\ -\frac{1}{2} - a_4 - c_2 \end{bmatrix} : a_4 = -\frac{1}{2}c_2 \pm \frac{1}{2}\sqrt{(1-3c_2)(1+c_2)}, -1 \leq c_2 \leq \frac{1}{3} \end{cases},$$

$$\mathcal{C}_2 = \begin{cases} \begin{bmatrix} \frac{1}{2} & a_4 \\ -\frac{1}{2} & -a_4 - c_2 \\ c_2 & -\frac{1}{2} + a_4 \\ -\frac{1}{2} - a_4 - c_2 \end{bmatrix} : a_4 = -\frac{1}{2}c_2 \pm \frac{1}{2}\sqrt{(1+3c_2)(1-c_2)}, -\frac{1}{3} \leq c_2 \leq 1 \end{cases}.$$  

It is to be noted that any matrix in $\mathcal{C}_1$ has row and column sums $-1$ while for $\mathcal{C}_2$ it is $1$. Also, matrices in $\mathcal{C}_1$ and $\mathcal{C}_2$ are linear sum of at most 6 permutation matrices.

Hence the proof. □
Remark 2.18. 1. Let $A \in \mathcal{L}$ be a $4 \times 4$ orthogonal matrix, such that $PAQ$ is the direct
sum of permutative orthogonal matrices for some $P, Q \in \mathcal{P}_4$. Then $PAQ = \begin{bmatrix} 1 & 0 \\ 0 & B \end{bmatrix}$ for

\[ B \in \mathcal{X}_1 \cup \mathcal{Z}_1, \text{ or } PAQ = \begin{bmatrix} -1 & 0 \\ 0 & C \end{bmatrix} \text{ for } C \in \mathcal{Y}_{-1} \cup \mathcal{W}_{-1}, \text{ where} \]

\[ \mathcal{X}_1 = \left\{ \begin{bmatrix} x & y & 1-x-y \\ 1-x-y & x & y \\ y & 1-x-y & x \end{bmatrix} : x^2 + y^2 - x - y + xy = 0 \right\}, \]

\[ \mathcal{Y}_{-1} = \left\{ \begin{bmatrix} x & y & -1-x-y \\ -1-x-y & x & y \\ y & -1-x-y & x \end{bmatrix} : x^2 + y^2 + x + y + xy = 0 \right\}, \]

$\mathcal{Z}_1 = \{ PA : A \in \mathcal{X}_1 \}, \mathcal{W}_{-1} = \{ PB : B \in \mathcal{Y}_{-1} \}$ and $P$ is the $3 \times 3$ permutation matrix

\[ \text{corresponds to the permutation (23). Note that union of } \mathcal{X}_1, \mathcal{Y}_{-1}, \mathcal{Z}_1 \text{ and } \mathcal{W}_{-1} \text{ provides} \]

the set of all permutative orthogonal matrices of order $3 \times 3$ [22]. Clearly if $PAQ$ is the
direct sum of two $2 \times 2$ permutative matrices, then $PAQ \in \mathcal{P}_4$ or equivalently $A \in \mathcal{P}_4$.

2. It follows from the characterization of all orthogonal matrices in $\mathcal{L}_1 \oplus \mathcal{L}_3 \oplus \mathcal{L}_4$ described
in Theorem 2.17 that: any orthogonal matrix in $\mathcal{L}_1 \oplus \mathcal{L}_3 \oplus \mathcal{L}_4$ need be permutative or
direct sum of permutative matrices but of specific form as described by $\mathcal{C}_1$ and $\mathcal{C}_2$.

3. Observe that any orthogonal matrix belongs to the space $\mathcal{L}_i \oplus \mathcal{L}_j \oplus \mathcal{L}_k$, $i, j, k \in \{1, \ldots, 5\}$,

$(i, j, k) \neq (1, 2, 5)$ has one parameter representation. Besides, each of the orthogonal
matrices can be written as a linear sum of at most 6 permutative matrices. However,
we are not able to characterize orthogonal matrices that belong to the space $\mathcal{L}_1 \oplus \mathcal{L}_2 \oplus \mathcal{L}_5$
of symmetric matrices using the straightforward approach as considered above. This can
happen due to the fact that the orthogonal matrices in this space need not be written as
linear sum of at most 6 permutations. For example, consider the following matrix:

\[ \frac{1}{11} \begin{bmatrix} 10 & -2 & -1 & 4 \\ -2 & 7 & -2 & 8 \\ -1 & -2 & 10 & 4 \\ 4 & 8 & 4 & -5 \end{bmatrix} = \frac{1}{11} P_{(12)} + \frac{7}{11} P_{(34)} - \frac{1}{11} P_{(13)(24)} + \frac{4}{11} P_{(14)(23)} + \frac{9}{11} P_{(24)} - \frac{3}{11} P_{(12)(34)} - \frac{6}{11} P_{(23)} \in \mathcal{L}_1 \oplus \mathcal{L}_2 \oplus \mathcal{L}_5. \]

3 Localization of two dimensional quantum walks

In this section we consider DTQWs on lattices when the coins are real permutative orthogonal matrices. In particular, we study the localization property of these walks at the initial position which is considered as the origin of the infinite lattice. First, we formally introduce the walk on a square two-dimensional lattice $Z_N$ as follows. The square lattice is defined as

\[ Z_N = \{(x, y) \in \mathbb{Z}^2 : -(N-1)/2 \leq x \leq (N-1)/2, -(N-1)/2 \leq y \leq (N-1)/2 \}, \]

where $\mathbb{Z}$ denotes the set of all integers. Obviously, $Z_N$ is the two-dimensional grid centered at the origin of the standard $XY$-plane and it contains $N^2$ vertices. Besides, note that $N$ is a positive odd integer.

The quantum walker on the lattice can have four directions of motion at a vertex that are
called chirality of the walker denoted by $|S\rangle$ where $S \in \{R, L, U, D\}; |R\rangle = |1\rangle, |L\rangle = |2\rangle,$

$|U\rangle = |3\rangle$ and $|D\rangle = |4\rangle$ stand for right, left, up and down respectively, and $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle \}$ is the canonical ordered orthonormal basis of the four-dimensional coin space $\mathcal{H}_c$. We denote

$1 \leq \ell(s) \leq 4$ as the ordering of the element $|S\rangle$ in the canonical basis. The $N^2$-dimensional position space $\mathcal{H}_p$ is given by the complex Hilbert space generated by the orthonormal basis
Thus the state space of the quantum walker is the $4N^2$-dimensional Hilbert space $\mathcal{H}_q \otimes \mathcal{H}_c$ generated by the orthonormal basis \{$(S, x, y) : S \in \{R, L, U, D\}, (x, y) \in \mathbb{Z}_N$\}. In what follows, we denote \$S, x, y, t \$ as the state of the quantum walker at a given vertex \$(x, y) \$ at time-step \$t \$ with coin state \$S \$. Thus the orthonormal basis of $\mathcal{H}_q \otimes \mathcal{H}_c$ that we consider in this paper is given by \$|S, x, y \rangle = |w' \rangle \$ where \$w' = 4N\gamma + 4x + l(S) + 2N^2 - 2 \$ and hence, \$\{|w' \rangle : 1 \leq w' \leq 4N^2 \}$ is the canonical orthonormal basis of the aforementioned $4N^2$ dimensional complex Hilbert space. Then the quantum state corresponding to the quantum walker at time \$t \$ can be written as
\[
|\psi(t)\rangle = \sum_{S \in \{R, L, U, D\}} \sum_{(x, y) \in \mathbb{Z}_N} \alpha_{S, x, y, t} |S, x, y, t\rangle.
\]

We denote
\[
|\psi_{x, y}(t)\rangle = \sum_{S \in \{R, L, U, D\}} \alpha_{S, x, y, t} |S\rangle
\]
which will be used in sequel.

Then the time-evolution of the state corresponding to a coin operator \$C = [c_{ij}] \$ is defined as
\[
|R, x, y, t + 1\rangle = c_{11} |R, x-1, y, t\rangle + c_{12} |L, x-1, y, t\rangle + c_{13} |U, x-1, y, t\rangle + c_{14} |D, x-1, y, t\rangle,
\]
\[
|L, x, y, t + 1\rangle = c_{21} |R, x+1, y, t\rangle + c_{22} |L, x+1, y, t\rangle + c_{23} |U, x+1, y, t\rangle + c_{24} |D, x+1, y, t\rangle,
\]
\[
|U, x, y, t + 1\rangle = c_{31} |R, x, y-1, t\rangle + c_{32} |L, x, y-1, t\rangle + c_{33} |U, x, y-1, t\rangle + c_{34} |D, x, y-1, t\rangle,
\]
\[
|D, x, y, t + 1\rangle = c_{41} |R, x, y+1, t\rangle + c_{42} |L, x, y+1, t\rangle + c_{43} |U, x, y+1, t\rangle + c_{44} |D, x, y+1, t\rangle,
\]
where \$(x, y) \in \mathbb{Z}_N \$ with periodic boundary condition [10]. If \$C = G \$, the Grover matrix (see equation (10)) the corresponding quantum walk is called the Grover walk. The walk can be described as \$|\psi(t)\rangle = U^t |\psi(0)\rangle \$, \$t \geq 1 \$ for some unitary evolution operator \$U = S_f(C \otimes I) \$ where \$S_f \$ is the shift operator, \$C \$ is the coin operator, and \$|\psi(t)\rangle \in \mathcal{H}_q \otimes \mathcal{H}_c \$ denotes the wave function of the walker at time \$t \$. The shift operator is defined as \$S_f = \sum_{(x, y) \in \mathbb{Z}_N} S_{x, y} \$ where \$S_{x, y} \$ acts as moving the position of the walking particle from the position at the vertex \$(x, y) \$ to one of the positions \$(x-1, y), (x+1, y), (x, y-1), (x, y+1) \$ depending on the coin state. Indeed,
\[
S_{x, y} = |R\rangle \langle R| \otimes |x-1\text{(mod}N)\rangle \langle x, y| + |L\rangle \langle L| \otimes |x+1\text{(mod}N)\rangle \langle x, y| + |U\rangle \langle U| \otimes |x, y-1\text{(mod}N)\rangle \langle x, y| + |D\rangle \langle D| \otimes |x, y+1\text{(mod}N)\rangle \langle x, y|,
\]
when \$N \$ is finite. Note that \$|x, y\rangle = |x\rangle \otimes |y\rangle \$.

Then the probability of finding the walker at a vertex \$(x, y) \$ at time \$t \$ is given by
\[
P_t((x, y); \psi(0)) = \|\psi_{x, y}(t)\|^2 = \sum_{S \in \{R, L, U, D\}} |\alpha_{S, x, y, t}|^2 = \sum_{S \in \{R, L, U, D\}} P_t(S, (x, y); \psi(0)),
\]
where the initial state \$\psi(0) \$ is known. The walk is called localized if the particle has a non-vanishing probability to stay at any position even in the limit of infinite number of steps [26], [15]. However, it is well known that \$P_t \$ does not converge, and hence its average over time is considered as follows [1]:
\[
\overline{P}_t((x, y); \psi(0)) = \frac{1}{T} \sum_{t=0}^{T-1} P_t((x, y); \psi(0)).
\]
Finally, the quantity \( P_t((x, y); \psi(0)) \) when \( T \to \infty \) captures the proportion of time which the walker “spends” in any given node \((x, y) \in \mathbb{Z}_N\) for any initial state \(\psi(0)\). Essentially, nonzero value of \(\lim_{T \to \infty} P_t((x, y); \psi(0))\) guarantees the localization at \((x, y) \in V(\mathbb{Z}_N)\) when \(N \to \infty\), that is, for infinite lattice [10].

It is well known that Grover walk shows localization property [10]. Moreover, the dependency of the behavior of walker is further analyzed to show that localization also depends on the initial position of the walker for long time intervals. It is shown in [10] that the localization of Grover walks happens due to the degeneration of eigenvalues of the time evolution operator. It is found that the eigenvalues of the evolution matrix \(U\) corresponding to the Grover walk can be derived from the eigenvalues of another matrix \(U_{n,m} = D_{n,m} G\) where \(D_{n,m}\) is a unitary diagonal matrix and \(G\) is the Grover matrix. It is not surprising that the same holds true when the Grover matrix is replaced by any coin operator, which we show in the following proposition for the completeness of our results. The proof is similar to the case when the coin operator is of dimension \(3 \times 3\) as considered in [22].

**Proposition 3.1.** The two dimensional quantum walk operator \(U = S_f(C \otimes I)\) has eigenvalues \(\lambda_{n,m,j}\) with a corresponding eigenvector \(|\eta_{n,m,j}\rangle = |\phi_n, \phi'_m\rangle\) where \(\lambda_{n,m,j}\) is an eigenvalue of \(U_{n,m} = D_{n,m} C\) corresponding to an eigenvector \(|\phi_{n,m,j}\rangle\), \(|\phi_n\rangle = \sum_{x = -N/2}^{N/2} e^{-ikx} |x\rangle\), and \(|\phi'_m\rangle = \sum_{y = -N/2}^{N/2} e^{-iky} |y\rangle\); \(k = 2\pi n / N, m \in \{0, 1, \ldots, N-1\}\), and \(D_{n,m} = \text{diag}(\omega^{-n}, \omega^{n}, \omega^{-m}, \omega^{m})\) where \(\omega = e^{2\pi i / N}\) for \(i = \sqrt{-1}\).

**Proof:** First, we consider the image of \(|j\rangle \otimes |\phi_{n,m}\rangle\) under \(S_f\). Then

\[
S_f(|R\rangle \otimes |\phi_n, \phi'_m\rangle) = \sum_{(x,y) \in \mathbb{Z}_N} S_{x,y}(|R\rangle \otimes |\phi_n, \phi'_m\rangle)
\]

\[
= |R\rangle \otimes \sum_{x = -(N-1)/2}^{(N-1)/2} e^{-ikx} |x \mod N, \phi'_m\rangle
\]

\[
= |R\rangle \otimes e^{-ik} \sum_{x = -(N-1)/2}^{(N-1)/2} e^{-ik(x-1)} |x \mod N, \phi'_m\rangle
\]

\[
= e^{-ik} |R\rangle \otimes |\phi_n, \phi'_m\rangle
\]

\[
= \omega^{-n} |R\rangle \otimes |\phi_n, \phi'_m\rangle
\]

Similarly, \(S_f(|L\rangle \otimes |\phi_n, \phi'_m\rangle) = \omega^n |L\rangle \otimes |\phi_n, \phi'_m\rangle, S_f(|U\rangle \otimes |\phi_n, \phi'_m\rangle) = \omega^{-m} |U\rangle \otimes |\phi_n, \phi'_m\rangle, S_f(|D\rangle \otimes |\phi_n, \phi'_m\rangle) = \omega^m |D\rangle \otimes |\phi_n, \phi'_m\rangle\).

Let \(|v_{n,m,j}\rangle\) be an eigenvector of \(U_{n,m}\) corresponding to the eigenvalue \(\lambda_{n,m,j}\). Let \(C|v_{n,m,j}\rangle = \sum_{j \in \{R, L, U, D\}} \alpha_j |j\rangle\) for some \(\alpha_j \in \mathbb{C}\). Then

\[
U|\eta_{n,m,j}\rangle = S_f(C|v_{n,m,j}\rangle \otimes |\phi_n, \phi'_m\rangle)
\]

\[
= (\omega^{-n}\alpha_R |R\rangle + \omega^n\alpha_L |L\rangle + \omega^{-m}\alpha_U |U\rangle + \omega^m\alpha_D |D\rangle) \otimes |\phi_n, \phi'_m\rangle
\]

\[
= D_{n,m} C|v_{n,m,j}\rangle \otimes |\phi_n, \phi'_m\rangle
\]

\[
= \lambda_{n,m,j} |\eta_{n,m,j}\rangle
\]

This completes the proof. □

Then the following corollary describes how to obtain each entry of eigenvectors of \(U\) from the eigenvectors of \(U_{n,m}\).

**Corollary 3.2.** Let \((\lambda_{n,m,k}, \eta_{n,m,k})\), \(k \in \{1, 2, 3, 4\}, \{0, 1, \ldots, N-1\}\) denote eigenpairs of \(U\). If \(\eta_{n,m,k} = |\eta_{r,n,m,k}\rangle, r = 1, \ldots, 4N^2\) then

\[
\eta_{r,n,m,k} = \frac{v_{x,n,m,k}(nx+my)}{N||v_{n,m,k}\rangle_2}
\]

18
where \((x, y) \in \mathbb{Z}_N\) and \(s \in \{1, 2, 3, 4\}\) satisfy \(r = 4Ny + 4x + s + 2N^2 - 2\) and \(v_{n,m,k} = [v_{s,n,m,k}]\) is an eigenvector of \(U_{n,m}\) associated with the eigenvalue \(\lambda_{n,m,k}\).

In next proposition we show that the eigenvectors of \(U\) as described in Proposition 3.1 are orthonormal.

**Proposition 3.3.** The eigenvectors \(|\eta_{n,m,k}\rangle, 1 \leq k \leq 4, 0 \leq m, n \leq N - 1\) of \(U\) form an orthonormal set.

**Proof:** First suppose \(\lambda_{n',m',k'} \neq \lambda_{n,m,k}\), so that \(|\langle \eta_{n',m',k'} | \eta_{n,m,k}\rangle| = 0\), since the eigenvectors of unitary matrices corresponding to different eigenvalues are orthogonal. Next consider the case for degenerate eigenvalues whenever \(\lambda_{n',m',k} = \lambda_{n,m,k}\). Then Using Corollary 3.2,

\[
\langle \eta_{n',m',k} | \eta_{n,m,k}\rangle = \sum_{r=1}^{4N^2} \bar{\eta}_{r,n',m',k} \eta_{r,n,m,k}
\]

\[
= \sum_{x,y \in \mathbb{Z}_N} \sum_{s=1}^{4} \bar{v}_{s,n',m',k} \omega^{(n'x + m'y)} v_{s,n,m,k} \omega^{-(nx + my)} \frac{1}{N \|v_{n,m,k}\|_2} \sum_{x,y} \omega^{(n'-n)x+(m'-m)y}
\]

\[
= \begin{cases} 
0, & \text{if } (n,m) \neq (n',m') \\
1, & \text{if } (n,m) = (n',m') 
\end{cases}
\]

since \(\sum_{x=-\frac{N-1}{2}}^{\frac{N-1}{2}} \omega^{ax} = \omega^{-\alpha} \sum_{x=0}^{N-1} \omega^{ax} = 0\) as \(\omega^N = e^{2\pi \alpha} = 1\). Hence the proof. \(\square\)

The numbers \(n\) and \(m\) in the above expressions are known as quantum numbers. We recall the observation from [10] that if the quantum walk exists initially at a vertex and all eigenvalues of evolution matrix are distinct then the probability of observing the quantum walk at the initial vertex goes to zero for infinite lattice. Thus, it is of utmost important to determine eigenvalues of \(U\) when the coin operator is a generalized Grover coin given by equation (11).

From Theorem 2.1 and Corollary 2.5 the one-parameter representation of the generalized Grover coins are given by \(C \in P_{(34)} Y_1 \cup P_{(24)} Y_1 \cup P_{(23)} Z_1\), where

\[
(P_{(34)} Y_1)_\theta = \begin{bmatrix} 
\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta \\
\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta \\
\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta \\
\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta 
\end{bmatrix} : \theta \in [-\pi, \pi] 
\]

\[
(P_{(24)} Y_1)_\theta = \begin{bmatrix} 
\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta \\
\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta \\
\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta \\
\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta 
\end{bmatrix} : \theta \in [-\pi, \pi] 
\]

\[
(P_{(23)} Z_1)_\theta = \begin{bmatrix} 
\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta \\
\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta \\
\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta \\
\frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta & \frac{1}{2} \sin \theta 
\end{bmatrix} : \theta \in [-\pi, \pi] 
\]

by setting \(z = \frac{1 + \cos \theta}{2}\) and hence \(x = \frac{\sin \theta}{2}\). Below we study the localization phenomena at initial position of the walker on the infinite lattice when the DTQWs are defined by generalized Grover coins and a class of permutative orthogonal matrices that does not contain the Grover coin. We mention that localization property of Grover walk on a finite lattice depends on the size of the lattice [10], and hence our primary concern in this paper is on infinite lattice.
3.1 With coins from \((P_{24})_\theta\)

In this section, we consider the proposed DTQWs when the coin operator \(C\) belongs to \((P_{24})_\theta\), \(\theta \neq \pi, -\pi\). Note that if \(U = S_f(C \otimes I)\) denotes the evolution operator then

\[
U_{n,m} = D_{n,m}C = \begin{bmatrix}
\frac{1}{2} \sin \theta \omega^{-n} & \frac{1+\cos \theta}{2} \omega^{-n} & -\frac{1}{2} \sin \theta \omega^{-n} & \frac{1-\cos \theta}{2} \omega^{-n} \\
\frac{1-\cos \theta}{2} \omega^{n} & \frac{1}{2} \sin \theta \omega^{n} & \frac{1+\cos \theta}{2} \omega^{n} & -\frac{1-\cos \theta}{2} \omega^{n} \\
-\frac{1}{2} \sin \theta \omega^{-m} & \frac{1+\cos \theta}{2} \omega^{-m} & \frac{1}{2} \sin \theta \omega^{-m} & \frac{1-\cos \theta}{2} \omega^{-m} \\
\frac{1-\cos \theta}{2} \omega^{m} & \frac{1}{2} \sin \theta \omega^{m} & \frac{1+\cos \theta}{2} \omega^{m} & -\frac{1-\cos \theta}{2} \omega^{m}
\end{bmatrix} \tag{20}
\]

where \(\theta \in (-\pi, \pi)\). First we derive the eigenvalues of \(U_{n,m}\) for \(n, m \in \{0, \ldots, N-1\}\) as follows.

Lemma 3.4. Consider \(U_{n,m}\) from equation (20). Then a complete set of orthogonal eigenpairs \((\lambda_{n,m,k}, v_{n,m,k})\), \(k = 1, \ldots, 4\) of \(U_{n,m}\) are

\[
\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = \frac{\sin \theta (\cos \zeta_n + \cos \zeta_m) + i \sqrt{4 - \sin^2 \theta (\cos \zeta_n + \cos \zeta_m)^2}}{2},
\]

\[
\lambda_{n,m,4} = \frac{\sin \theta (\cos \zeta_n + \cos \zeta_m) + i \sqrt{4 - \sin^2 \theta (\cos \zeta_n + \cos \zeta_m)^2}}{2},
\]

\[
v_{n,0,k} = \begin{cases} 
(1 + \cos \theta + \sin \theta) \omega^{-n} & (1 + \cos \theta + \sin \theta) \omega^{-n} & 1 & -1 \end{cases}^T \text{ if } k = 1
\]

\[
(1 + \cos \theta) \omega^{-n} + \sin \theta & (1 + \cos \theta) \omega^{-n} + \sin \theta & 1 & 1 \end{cases}^T \text{ if } k = 2
\]

\[
(1 + \cos \theta) \omega^{-n} - \sin \theta & (1 + \cos \theta) \omega^{-n} - \sin \theta & 1 & 1 \end{cases}^T \text{ if } k = 2
\]

\[
(1 + \cos \theta) \omega^{-n} - \sin \theta & (1 + \cos \theta) \omega^{-n} - \sin \theta & 1 & 1 \end{cases}^T \text{ if } k = 2
\]

\[
(1 - \cos \theta) \lambda_{n,0,k} \omega^{-n} + \sin \theta & (1 + \cos \theta) \lambda_{n,0,k} \omega^{-n} - \sin \theta & 1 & 1 \end{cases}^T \text{ if } k = 3, 4
\]

if \(n > 0\), and

\[
v_{n,m,k} = \begin{bmatrix} (1 + \cos \theta) \lambda_{n,m,k} \omega^{-n} - \sin \theta \\ (1 - \cos \theta) \lambda_{n,m,k} \omega^{-n} + \sin \theta \\ 1 + \cos \theta - \lambda_{n,m,k} \sin \theta \omega^m \\ (1 + \cos \theta) \lambda_{n,m,k} \omega^{-n} - \sin \theta \end{bmatrix}^T \text{ if } k = 1
\]

\[
(1 + \cos \theta) \lambda_{n,m,k} \omega^{-n} - \sin \theta & (1 + \cos \theta) \lambda_{n,m,k} \omega^{-n} - \sin \theta & 1 & 1 \end{cases}^T \text{ if } k = 2
\]

\[
(1 + \cos \theta) \lambda_{n,m,k} \omega^{-n} - \sin \theta & (1 + \cos \theta) \lambda_{n,m,k} \omega^{-n} - \sin \theta & 1 & 1 \end{cases}^T \text{ if } k = 2
\]

\[
(1 + \cos \theta) \lambda_{n,m,k} \omega^{-n} - \sin \theta & (1 + \cos \theta) \lambda_{n,m,k} \omega^{-n} - \sin \theta & 1 & 1 \end{cases}^T \text{ if } k = 2
\]

if \(n, m > 0\) and \(k \in \{1, 2, 3, 4\}\), where \(\zeta_q = 2\pi q/N, q \in \{m,n\}\).

Proof: Note that \(\omega^q = e^{i \zeta_q}\). We also note that the characteristic polynomial of \(U_{n,m}\) is given by

\[
\chi_{U_{n,m}}(\lambda) = \lambda^4 - \sin \theta (\cos \zeta_n + \cos \zeta_m) \lambda^3 + \sin \theta (\cos \zeta_m + \cos \zeta_n) \lambda - 1.
\]

By calculating the roots, we get the eigenvalues and the corresponding eigenvectors can be obtained by solving the system of equations \((U_{n,m} - \lambda_{n,m,k}I)X = 0\) for \(X\). Since \(U_{n,m}\) is a unitary matrix, eigenvectors of \(U_{n,m}\) corresponding to different eigenvalues are orthogonal. □

By Proposition 3.3, \(|\eta_{n,m,k}\rangle, 1 \leq k \leq 4, 0 \leq m, n \leq N - 1\) are the set of orthonormal eigenvectors corresponding to the eigenvalue \(\lambda_{n,m,k}\) of \(U\). Thus

\[
U = \sum_{n,m,k} \lambda_{n,m,k} |\eta_{n,m,k}\rangle \langle \eta_{n,m,k}|
\]
Consequently,

\[ |\psi(t)\rangle = U^t |\psi(0)\rangle = \sum_{n,m,k} \lambda_{n,m,k}^t |\eta_{n,m,k}\rangle \langle \eta_{n,m,k} |\psi(0)\rangle \]

\[ = \sum_{j=1}^{4N^2} \sum_{n,m,k} \lambda_{n,m,k}^j \bar{\eta}_{j,n,m,k} \psi_j(0) |\eta_{n,m,k}\rangle \]

\[ = \sum_{j=1}^{4N^2} \sum_{n,m,k} \lambda_{n,m,k}^j \bar{\eta}_{j,n,m,k} \psi_j(0) \eta_{r,n,m,k} |S, x, y, t\rangle, \]

where \( r = 4NY + 4x + l(S) + 2N^2 - 2 \). Then since the eigenvectors of the proposed evolution operator \( U \) can be obtained by the eigenvectors of \( U_{n,m} \) derived in Lemma 3.4, the wave function of the proposed DTWQ can be obtained by employing Corollary 3.2. Indeed,

\[ |\psi(t)\rangle = \sum_{S \in \{R, L, U, D\}} \sum_{(x,y) \in Z_N} \alpha_{|S,x,y,t\rangle} |S, x, y, t\rangle \]

where

\[ \alpha_{|S,x,y,t\rangle} = \sum_{j=1}^{4N^2} \sum_{n,m,k} \lambda_{n,m,k}^j \bar{\eta}_{j,n,m,k} \psi_j(0) \eta_{r,n,m,k} \] (21)

where \( j = 4NY' + 4x' + l(S') + 2N^2 - 2 \), and \( \psi_j(0) = \alpha_{|S',x',y',0\rangle}, (x', y') \in Z_N, S' \in \{R, L, U, D\}. \)

Using equations (14) and (21) we have

\[ |\psi_{x,y}(t)\rangle = \sum_{n,m,k} \lambda_{n,m,k}^t \bar{v}_{n,m,k} \psi_{0,0}(0) \frac{1}{N^2 \|v_{n,m,k}\|^2} v_{n,m,k} \omega^{-\omega_{nx+my}}. \]

and consequently, \( P_t((x,y); |\psi(0)\rangle) = \sum_{S \in \{R, L, U, D\}} |\alpha_{|S,x,y,t\rangle}|^2 = \|\psi_{x,y}(t)\|^2 \) follows from equation (15). However, an analytical expression of it would be hard to obtain due to the cumbersome expressions of eigenvectors \( v_{n,m,k} \) of \( U_{n,m} \) given by Lemma 3.4.

We now consider calculating the total time-averaged probability for finding the walker at the initial position when the lattice is infinite. We follows [10] to analyze the localization property of the proposed DTQWs. We show that precise value of the time-averaged probability is hard to obtain and we provide a computable integral formula for time-averaged probability when the initial coin states are basis states letting \( N \to \infty \). Then fixing the initial coin state we plot the total time-averaged probability for the walker to be found at the initial position, the origin of the infinite two-dimensional lattice for several generalized Grover coins.

Recall from equations (15)-(16) that the time-averaged probability such that the walker can be found at a vertex \((x, y) \in Z_N\) is given by

\[ P_t((x, y); \psi(0)) = \frac{1}{T} \sum_{t=0}^{T-1} \sum_{S \in \{R, L, U, D\}} |\alpha_{|S,x,y,t\rangle}|^2, \] (22)

where \( |\psi(0)\rangle \) denotes the initial state of the wave function. Now we introduce some notations that enable us to derive a compact expression of \( P_t((x, y); \psi(0)) \) utilizing the fact that eigenvalues of \( U \) are repeated for different pairs of \((n, m)\). We refer to different terms of \( \alpha_{|S,x,y,t\rangle} \) given in equation (21) as follows:

\[ c_{r,j,0,0,k} = \frac{\omega_{|S(0,0,0,0),l(S'),0,0,k\rangle}}{\|\omega_{0,0,0}\|^2}, \quad c_{r,j,n,m,k} = \sum_{(n',m') \in \Omega(n,m)} \frac{\omega_{|S(n',m'),l(S'),0,0,k\rangle}}{\|\omega_{n',m',0}\|^2} \] (23)

21
where the second expression is defined for \( n > 0 \) and \( m > 0 \), and \( \Omega(n, m) = \{(n', m') : \Lambda(U_{n, m}) = \Lambda(U_{n', m'})\} \), \( \Lambda(X) \) denotes the spectrum of a matrix \( X \). Indeed, \( \Omega(n, m) = \{(n, 0), (0, n), (N - n, 0), (0, N - n)\} \) if \( m = 0 \); \( \Omega(n, m) = \{(n, n), (n, N - n), (N - n, n), (N - n, N - n)\} \) if \( n = m \); and \( \Omega(n, m) = \{(n, n), (n, N - m), (N - n, m), (m, n), (m, N - n), (N - m, n), (N - m, N - n)\} \) otherwise; follows from the fact that \( \cos \zeta_n + \cos \zeta_m = \cos \zeta_n + \cos \zeta_m \) when \( (n', m') \in \Omega(n, m) \), \( \zeta_q = 2\pi q/N, q \in \{n, m\} \).

Thus from (21) we obtain

\[
\alpha_{\{S, x, y, t\}} = \frac{1}{N^2} \sum_{j=1}^{4N^2} C_{r,j,1}(-1)^j + C_{r,j,2} + \sum_{n=1}^{N-1} \sum_{k=3}^{4} c_{r,j,n,0,k} \lambda_{n,0,k}^{\prime} + \sum_{n=1}^{N-1} \sum_{m=1}^{N-1} \sum_{k=3}^{4} c_{r,j,n,m,k} \lambda_{n,m,k}^{\prime},
\]

(24)

where

\[
C_{r,j,1} = \sum_{k=1}^{3} c_{r,j,0,0,k} + \sum_{n=1}^{N-1} c_{r,j,n,0,1} + \sum_{n=1}^{N-1} c_{r,j,n,n,1} + \sum_{n=1}^{N-3} \sum_{m=1}^{N-1} c_{r,j,n,m,1},
\]

(25)

\[
C_{r,j,2} = c_{r,j,0,0,2} + \sum_{n=1}^{N-1} c_{r,j,n,0,2} + \sum_{n=1}^{N-1} c_{r,j,n,n,2} + \sum_{n=1}^{N-3} \sum_{m=1}^{N-1} c_{r,j,n,m,2}.
\]

(26)

In what follows, we determine the time-averaged probability \( \overline{P}(x, y; \psi(0)) \) of the proposed DTQWs when \( T \to \infty \) and the walker’s initial position is at \((0, 0)\) with initial coin state \(|S\rangle\), \( S \in \{R, L, U, D\} \). Thus we denote the time-averaged probability that the walker can be found at \((0, 0)\) with state \( S' \in \{R, L, U, D\} \) as

\[
\overline{P}(S', (0, 0); \psi_S(0)) = \lim_{T \to \infty} \frac{1}{T} \sum_{t=0}^{T-1} |\alpha_{\{S', 0,0,t\}}|^2
\]

(27)

where \(|\psi_S(0)\rangle \in H_p \otimes H_c\) denotes the initial state of the walker with \(|S\rangle\) as the initial coin state when the walk is defined on the finite lattice with vertex set \( Z_N \). It can be checked that if \(|\psi_S(0)\rangle = |\psi_j(0)\rangle\), \( 1 \leq j \leq 4N^2 \) then \( \psi_j(0) = 1 \) when \( j = l(S) + 2N^2 - 2 \) and \( \psi_j(0) = 0 \) otherwise. Later we derive

\[
\overline{P}_\infty(\psi_S(0), S') = \lim_{N \to \infty} \overline{P}(S', (0, 0); \psi_S(0)), S' \in \{R, L, U, D\}
\]

that is, the time-averaged probability of the walker to be found at \((0, 0)\) on the infinite lattice. Then finally we compute the total time-averaged probability of finding the walker at \((0, 0)\), that is

\[
\overline{P}_\infty(\psi_S) = \sum_{S' \in \{R, L, U, D\}} \overline{P}_\infty(\psi_S, S'),
\]

(27)

which captures the proportion of time that the walker spends at the initial position \((0, 0)\).

First we have the following lemma.

**Lemma 3.5.** Let \( \lambda_{n,m,k} \neq \lambda_{n', m', k'} \) be two eigenvalues of \( U \). Then

\[
\lim_{T \to \infty} \frac{1}{T} \sum_{t=0}^{T-1} (\lambda_{n,m,k})^t (\overline{\lambda}_{n', m', k'})^t = 0.
\]
Proof: Let \(\lambda_{n,m,k} = e^{i\theta}\) and \(\lambda'_{n',m',k'} = e^{i\theta'}\), \(\theta, \theta' \in \mathbb{R}\) and \(\theta - \theta' \neq 0, 2\pi, -2\pi\). Then

\[
\lim_{T \to \infty} \sum_{t=0}^{T-1} \frac{(\lambda_{n,m,k})^t(\lambda'_{n',m',k'})^t}{T} = \lim_{T \to \infty} \sum_{t=0}^{T-1} \frac{e^{i(\theta-\theta')t}}{T} = \lim_{T \to \infty} \frac{1 - e^{i(\theta'-\theta)T}}{T(1 - e^{i(\theta'-\theta)})} = \frac{1}{(1 - e^{i(\theta'-\theta)})} \lim_{T \to \infty} \frac{1 - e^{i(\theta'-\theta)T}}{T} = 0
\]

since \(\lim_{x \to \infty} \frac{\sin x}{x} = 0, \lim_{x \to \infty} \frac{\cos x}{x} = 0\). This completes the proof. \(\square\)

Then by Lemma 3.5 and equation (24), we obtain

\[
\overline{P}(S', (0,0); \psi_S(0)) = \frac{1}{N^4} \left[ \sum_{j=1}^{4N^2} \left| C_{r,j,1} \right|^2 + \sum_{j=1}^{4N^2} \left| C_{r,j,2} \right|^2 \right. \\
+ \sum_{n=1}^{N-1} \sum_{k=3}^{N-1} \sum_{j=1}^{4N^2} \left| C_{r,j,n,0,k} \right|^2 + \sum_{n=1}^{N-1} \sum_{k=3}^{N-1} \sum_{j=1}^{4N^2} \left| C_{r,j,n,n,k} \right|^2 \\
+ \sum_{n=1}^{N-1} \sum_{m=n+1}^{N-1} \sum_{k=3}^{N-1} \sum_{j=1}^{4N^2} \left| C_{r,j,n,m,k} \right|^2 \left. \right] .
\]

(28)

Note that the 3-rd and 4-th terms in the expression of \(\overline{P}(S', (0,0); \psi_S(0))\) are of order \(N^{-3}\), and the 5-th term is of order is \(N^{-2}\). Thus all these terms vanish when \(N \to \infty\) and we obtain

\[
\overline{P}_\infty(\psi_S(0), S') = \lim_{N \to \infty} \frac{1}{N^4} \left( \left| \sum_{j=1}^{4N^2} C_{r,j,1} \right|^2 + \left| \sum_{j=1}^{4N^2} C_{r,j,2} \right|^2 \right)
\]

\[= \lim_{N \to \infty} \frac{1}{N^4} \left( \left| C_{r,j,1} \right|^2 + \left| C_{r,j,2} \right|^2 \right),
\]

(29) where \(S, S' \in \{R, L, U, D\}\) and \(r = l(S') + 2N^2 - 2, j = l(S) + 2N^2 - 2\).

Then we have the following theorem which describes the time-averaged probability for finding the walker on the infinite lattice at the initial position \((0,0)\) with coin state \(|S'\rangle\) when the initial coin state is \(|S\rangle\).

**Theorem 3.6.** \(\overline{P}_\infty(\psi_S(0), S') = \frac{1}{8}\) if \(S = S' \in \{R, L, U, D\}\).

**Proof:** Let \(|S\rangle = |S'\rangle = |R\rangle\). Note that, if \(|\psi_R(0)\rangle = |\psi_j(0)\rangle, 1 \leq j \leq 4N^2\) then \(\psi_{2N^2-1}(0) = 1\) and \(\psi_j(0) = 0\) if \(j \neq 2N^2 - 1\). Then by equations (25), (26) and (29) we have

\[
\overline{P}_\infty(\psi_R(0), R) = \lim_{N \to \infty} \frac{1}{N^4} \left( \left| C_{r,j,1} \right|^2 + \left| C_{r,j,2} \right|^2 \right)
\]

\[= \lim_{N \to \infty} \frac{1}{N^4} \left( \sum_{n=1}^{(N-3)/2} \sum_{m=n+1}^{(N-1)/2} \sum_{j=1}^{4N^2} \left| C_{r,j,n,m,1} \right|^2 + \left| C_{r,j,n,m,2} \right|^2 \right).\]

\(r, j = 2N^2 - 1\).
Clearly the constant and single summation terms in $\text{Cr},j,1$ and $\text{Cr},j,1$ vanish while $N \to \infty$ in the above expression. Now from Theorem 3.2 we have

\[
v_{n,m,1} = \left[ \frac{(1 + \cos \theta + \sin \theta \omega^m)\omega^{-n}}{(1 + \cos \theta)\omega^{-n} + \sin \theta}, \frac{(1 + \cos \theta + \sin \theta \omega^m)}{(1 + \cos \theta)\omega^{-n} + \sin \theta}, 1, -\omega^m \right]^T,
\]

\[
v_{n,m,2} = \left[ \frac{(1 + \cos \theta - \sin \theta \omega^m)\omega^{-n}}{(1 + \cos \theta)\omega^{-n} - \sin \theta}, \frac{(1 + \cos \theta - \sin \theta \omega^m)}{(1 + \cos \theta)\omega^{-n} - \sin \theta}, 1, \omega^m \right]^T.
\]

Thus using equation (23) we have $c_{r,j,n,m,1} = c_{r,j,n,m,2} = 2.$ where $r, j = 2N^2 - 1.$ Hence

\[
P_\infty(\psi_R(0), R) = \lim_{N \to \infty} \frac{2}{N^4} \left[ \sum_{n=1}^{(N-3)/2} \sum_{m=n+1}^{(N-1)/2} 2 \right] = 2 \lim_{N \to \infty} \frac{1}{N^4} \left( \frac{(N - 1)(N - 3)}{2} \right)^2 = \frac{1}{8}.
\]

Similarly the proof follows for other cases. \hfill \square

Next we consider finding $P_\infty(\psi_S(0), S')$ when $S \neq S'$. Indeed note that it ultimately boils down computing the constants $c_{r,j,n,m,k}$ as follows. From equation (29) we have

\[
P_\infty(\psi_S(0), S') = \lim_{N \to \infty} \frac{1}{N^4} \left[ |Cr,j,1|^2 + |Cr,j,2|^2 \right]
\]

\[
= \lim_{N \to \infty} \frac{1}{N^4} \left( \sum_{n=1}^{N+1} \sum_{m=n+1}^{N+1} c_{r,j,n,m,1} \right)^2 + \left( \sum_{n=1}^{N+1} \sum_{m=n+1}^{N+1} c_{r,j,n,m,2} \right)^2,
\]

where $S, S' \in \{R, L, U, D\}$ and $r = l(S') + 2N^2 - 2, j = l(S) + 2N^2 - 2.$ Now from equation (23) we have

\[
c_{r,j,n,m,k} = \sum_{(n', m') \in \Omega, m < m'} \frac{v_{l(S'), n', m', k} V_{l(S), n', m', k}}{\|v_{n', m', k}\|^2}, k = 1, 2,
\]

whose values can be obtained by placing the values of $v_{l(S), n', m', k}$ and $v_{l(S'), n', m', k}$ from Lemma 3.4, where $r = l(S') + 2N^2 - 2$ and $j = l(S) + 2N^2 - 2, 1 \leq l(S), l(S') \leq 4.$ Indeed,

\[
c_{r,j,n,m,1} = \begin{cases} 
-2 (\cos \zeta_n + \cos \zeta_m + 2 \sin \theta \cos \zeta_n \cos \zeta_m) & \text{if } \{l(S), l(S')\} \in \{(1, 2), (3, 4)\}, l(S) \neq l(S'), \\
2 (1 + \cos \theta + (1 - \cos \theta) \cos \zeta_n \cos \zeta_m + \sin \theta (\cos \zeta_n + \cos \zeta_m)) & \text{if } l(S), l(S') \in \{1, 3\}, l(S) \neq l(S'), \\
-2 (\cos \zeta_n + \cos \zeta_m + \sin \theta (\cos \zeta_n + \cos \zeta_m)) & \text{if } \{l(S), l(S')\} \in \{(1, 4), (2, 3)\}, l(S) \neq l(S'), \\
2 ((1 + \cos \theta) \cos \zeta_n \cos \zeta_m + (1 - \cos \theta) + \sin \theta (\cos \zeta_n + \cos \zeta_m)) & \text{if } l(S), l(S') \in \{2, 4\}, l(S) \neq l(S'), \\
\end{cases}
\]

\[
c_{r,j,n,m,2} = \begin{cases} 
2 (\cos \zeta_n + \cos \zeta_m - 2 \sin \theta \cos \zeta_n \cos \zeta_m) & \text{if } \{l(S), l(S')\} \in \{(1, 2), (3, 4)\}, l(S) \neq l(S'), \\
2 (1 + \cos \theta + (1 - \cos \theta) \cos \zeta_n \cos \zeta_m - \sin \theta (\cos \zeta_n + \cos \zeta_m)) & \text{if } l(S), l(S') \in \{1, 3\}, l(S) \neq l(S'), \\
2 (\cos \zeta_n + \cos \zeta_m - 2 \sin \theta (\cos \zeta_n + \cos \zeta_m)) & \text{if } \{l(S), l(S')\} \in \{(1, 4), (2, 3)\}, l(S) \neq l(S'), \\
2 ((1 + \cos \theta) \cos \zeta_n \cos \zeta_m - (1 - \cos \theta) - \sin \theta (\cos \zeta_n + \cos \zeta_m)) & \text{if } l(S), l(S') \in \{2, 4\}, l(S) \neq l(S'). \\
\end{cases}
\]

Observe that due to complicated expressions of $c_{r,j,n,m,k}, k = 1, 2$ it is not feasible to come up with a value for $P_\infty(\psi_S(0), S')$ when $S \neq S'$ for all $\theta \in (-\pi, \pi)$. However as $N \to \infty,$
the limiting value for the sum of $c_{r,j,n,m,k}$ can be approximated by Riemann integration. For example, consider of $c_{r,j,n,m,1}$ where $l(S), l(S') \in \{1, 2\}, l(S) \neq l(S')$. Then,

$$\lim_{N \to \infty} \frac{1}{N^2} \sum_{n=1}^{N-1} \sum_{m=n+1}^{N-1} c_{r,j,n,m,1} = \frac{1}{8\pi^2} \int_{0}^{\pi} \int_{0}^{\pi} -\frac{2(cos x + cos y + 2 sin \theta cos x cos y)}{2 + sin(\theta cos x + cos y)} \, dx \, dy.$$

Now the values of $\overline{P}_\infty(\psi_S(0))$, $S \in \{R, L, U, D\}$ can be obtained using equation (27) after evaluating the Riemann integration for specific values of $\theta$. In Figure 1 we plot $\overline{P}_\infty(\psi_S(0))$ for different values of $\theta$ obtained by discretizing the interval $(-\pi, \pi)$ into 400 equidistant points. Note that, if $|\psi_S(0)| = |\psi_j(0)|$ then $\psi_j(0) = 1$ if $j = l(S) + 2N^2 - 2$ and 0 otherwise. The total time-averaged probabilities $\overline{P}_\infty(\psi_R), \overline{P}_\infty(\psi_U)$ are decreasing in contrast with $\overline{P}_\infty(\psi_L), \overline{P}_\infty(\psi_D)$, which are gradually increasing. Hence we conclude that the proposed DTQWs with canonical initial symmetric with respect to the vertical axis passing through $0$. When absolute value of $\theta$ is increasing $\overline{P}_\infty(\psi_R), \overline{P}_\infty(\psi_U)$ are decreasing in contrast with $\overline{P}_\infty(\psi_L), \overline{P}_\infty(\psi_D)$, which are gradually increasing. Hence we conclude that the proposed DTQWs with canonical initial states on infinite lattice localize when the initial position is $(0, 0)$. A similar analysis can be performed for any vertex $(x, y) \in Z_N$ as an initial position.

![Figure 1](image-url)

(a) $\overline{P}_\infty(\psi_R), \overline{P}_\infty(\psi_U)$ (b) $\overline{P}_\infty(\psi_L), \overline{P}_\infty(\psi_D)$

Figure 1: Numerical values of $\overline{P}_\infty(\psi_S), S \in \{R, L, U, D\}$ when the coins belong to $(P_{(24)}X_1)_\theta$ with 400 equidistant values of $\theta$ in $(-\pi, \pi)$.

### 3.2 With coins from $(P_{(34)}X_1)_\theta$ and $(P_{(23)}Z_1)_\theta$

In this section, we consider DTQWs when the coin operators $C'$ and $C''$ belong to $(P_{(34)}X_1)_\theta$, and $(P_{(23)}Z_1)_\theta$ respectively for $\theta \in (-\pi, \pi)$. Then

$$U'_{n,m} = D_{n,m}C' = \begin{bmatrix}
  \frac{1}{2} \sin \theta \omega^{-n} & -\frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} (1 + \cos \theta) \omega^{-n} & \frac{1}{2} (1 - \cos \theta) \omega^{-n} \\
  -\frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} \sin \theta \omega^{n} & -\frac{1}{2} (1 - \cos \theta) \omega^{n} & -\frac{1}{2} (1 + \cos \theta) \omega^{n} \\
  \frac{1}{2} (1 - \cos \theta) \omega^{-m} & \frac{1}{2} (1 + \cos \theta) \omega^{-m} & \frac{1}{2} \sin \theta \omega^{-m} & -\frac{1}{2} \sin \theta \omega^{-m} \\
  \frac{1}{2} (1 + \cos \theta) \omega^{m} & \frac{1}{2} (1 - \cos \theta) \omega^{m} & -\frac{1}{2} \sin \theta \omega^{m} & \frac{1}{2} \sin \theta \omega^{m}
\end{bmatrix},$$

and

$$U''_{n,m} = D_{n,m}C'' = \begin{bmatrix}
  \frac{1}{2} \sin \theta \omega^{-n} & \frac{1}{2} (1 + \cos \theta) \omega^{-n} & -\frac{1}{2} (1 - \cos \theta) \omega^{-n} & -\frac{1}{2} \sin \theta \omega^{-n} \\
  \frac{1}{2} (1 - \cos \theta) \omega^{n} & \frac{1}{2} \sin \theta \omega^{n} & \frac{1}{2} (1 + \cos \theta) \omega^{n} & \frac{1}{2} (1 - \cos \theta) \omega^{n} \\
  -\frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} (1 + \cos \theta) \omega^{-m} & -\frac{1}{2} \sin \theta \omega^{-m} & \frac{1}{2} (1 + \cos \theta) \omega^{-m} \\
  -\frac{1}{2} (1 - \cos \theta) \omega^{m} & \frac{1}{2} \sin \theta \omega^{m} & \frac{1}{2} (1 - \cos \theta) \omega^{m} & \frac{1}{2} (1 + \cos \theta) \omega^{m}
\end{bmatrix},$$

where $\theta \in [-\pi, \pi]$ and $D_{n,m} = \text{diag}(\omega^{-n}, \omega^{n}, \omega^{-m}, \omega^{m})$, $\omega = e^{2\pi i/N}$, $m, n \in \{0, \ldots, N - 1\}$. 

25
Recall that $(Y_k)_{\theta}, (Z_k)_{\theta}$ are permutationally similar to $(X_k)_{\theta}$. Indeed, $(Y_k)_{\theta} = P(23)(X_k)_{\theta}P(23)$ and $(Z_k)_{\theta} = P(13)(X_k)_{\theta}P(13)$ for $k = 1, \ldots, 4$. First we determine the eigenpairs of the unitary operators $U'_{n,m}$ and $U''_{n,m}$ as follows.

Lemma 3.7. A set of eigenpairs $(\lambda_{n,m,k}, v'_n, m_k)$, $k = 1, 2, 3, 4$ of $U'_{n,m}$ are given by

\[
\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = \sin \theta (\cos \zeta_n + \cos \zeta_m) - i \sqrt{4 - \sin^2 \theta (\cos \zeta_n + \cos \zeta_m)^2},
\]

\[
\lambda_{n,m,4} = \frac{\sin \theta (\cos \zeta_n + \cos \zeta_m) + i \sqrt{4 - \sin^2 \theta (\cos \zeta_n + \cos \zeta_m)^2}}{2},
\]

and

\[
v'_{n,m,k} = \begin{bmatrix}
\left( \sin \theta - (1 - \cos \theta) \lambda_{n,m,k} \omega^{-n} \right) \\
\left( 1 - \cos \theta \right) - \sin \theta \lambda_{n,m,k} \omega^m
\end{bmatrix} T
\]

where $\zeta_q = 2\pi q/N$ and $\omega^q = e^{i \zeta_q}$, $q \in \{m, n\}$.

Proof: The proof follows from the fact that the characteristic polynomial of $U'_{n,m}$ is $\chi_{U'_{n,m}}(\lambda) = \lambda^4 - \sin \theta (\cos \zeta_m + \cos \zeta_n) \lambda^3 + \sin \theta (\cos \zeta_m + \cos \zeta_n) \lambda - 1$.

Lemma 3.8. A set of eigenpairs $(\lambda_{n,m,k}, v''_n, m_k)$, $k = 1, 2, 3, 4$ of $U''_{n,m}$ are given by

\[
\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = \frac{\sin \theta (\cos \zeta_n + \cos \zeta_m) - i \sqrt{4 - \sin^2 \theta (\cos \zeta_n + \cos \zeta_m)^2}}{2},
\]

\[
\lambda_{n,m,4} = \frac{\sin \theta (\cos \zeta_n + \cos \zeta_m) + i \sqrt{4 - \sin^2 \theta (\cos \zeta_n + \cos \zeta_m)^2}}{2},
\]

and

\[
v''_{n,m,k} = \begin{bmatrix}
\left( \sin \theta - (1 + \cos \theta) \lambda_{n,m,k} \omega^m \right) \\
\left( 1 + \cos \theta \right) - \sin \theta \lambda_{n,m,k} \omega^{-m}
\end{bmatrix} T
\]

where $\zeta_q = 2\pi q/N$ and $\omega^q = e^{i \zeta_q}$, $q \in \{m, n\}$.

Proof: The proof follows from the fact that the characteristic polynomial of $U''_{n,m}$ is $\chi_{U''_{n,m}}(\lambda) = \lambda^4 - \sin \theta (\cos \zeta_m + \cos \zeta_n) \lambda^3 + \sin \theta (\cos \zeta_m + \cos \zeta_n) \lambda - 1$.

Note that $\Lambda(U_{n,m}) = \Lambda(U'_{n,m}) = \Lambda(U''_{n,m})$. Besides, a set of orthonormal eigenvectors of the evolution matrix corresponding to the DTQWs defined by generalized Grover coins in $(P_{(14)} X_1)_{\theta}$ and $(P_{(23)} Z_1)_{\theta}$ can be obtained by employing similar arguments as in the previous section. Thus an integration formula of time-average probabilities can be determined for these walks. Indeed, recall from (29) that

\[
P_\infty(\psi_S(0), S') = \lim_{N \to \infty} \frac{1}{N^2} \left( \sum_{n=1}^{(N-3)/2} \sum_{m=n+1}^{(N-1)/2} c_{r,j,n,m,1}^2 + \sum_{n=1}^{(N-3)/2} \sum_{m=n+1}^{(N-1)/2} c_{r,j,n,m,2}^2 \right).
\]
The values of \( c_{r,j,n,m,k,k} = 1,2 \) can be calculated using equation (23).

It may be noted that explicit expressions of \( c_{r,j,n,m,k,k} = 1,2 \) for different \( r \) and \( j \) is complicated. Thus we perform numerical computations for the values of

\[
\mathcal{P}_\infty(\psi_S) = \sum_{S' \in \{R,L,U,D\}} \mathcal{P}_\infty(\psi_S(0), S')
\]

for specific values of \( \theta \). We find that \( c_{r,j,n,m,k} \) are same for some pairs \((r,j)\), for example \( c_{1,3,n,m,k} = c_{1,4,n,m,k} = c_{2,3,n,m,k} = c_{2,4,n,m,k}, c_{1,2,n,m,k} = c_{3,4,n,m,k}, c_{1,1,n,m,k} = c_{2,2,n,m,k} = c_{3,3,n,m,k} = c_{4,4,n,m,k} \) which finally results in \( \mathcal{P}_\infty(\psi_S) \) to be same for all \( S \in \{R,L,U,D\} \) since \( c_{r,j,n,m,k} = c_{j,r,n,m,k} \), when the coin operator belongs to \((P_{34}(X_1))^\theta\). We plot \( \mathcal{P}_\infty(\psi_R(0)) \) considering 400 equidistant values of \( \theta \) in the interval \((-\pi, \pi)\) in Figure 2. It can be further observed from Figure 2 that the probability distribution \( \mathcal{P}_\infty(\psi_R) \) is symmetric with respect to the vertical axis through \( \theta = 0 \). Probabilities are maximum at \( \theta = \pi/2, -\pi/2 \). Finally, we conclude the DTQWs defined by the generalized Grover coins corresponding to these values of \( \theta \) localize at the initial position \((0,0)\) of the infinite lattice.

Figure 2: Numerical values of \( \mathcal{P}_\infty(\psi_S), S \in \{R,L,U,D\} \) when the coins belong to \((P_{34}(X_1))^\theta\) with 400 equidistant values of \( \theta \) in \((-\pi, \pi)\).

Next we plot the total time-average probabilities in Figure 3 for canonical initial coin states when the coin operator is in \((P_{23}(X_1)^\theta\), for different values of \( \theta \) obtained by discretizing the interval \((-\pi, \pi)\) into 400 equidistant points. Observe that, \( \mathcal{P}_\infty(\psi_S), S \in \{R,L,U,D\} \) are symmetric with respect to the vertical axis \( \theta = 0 \) and the time-average probability decreases or increases depending on the initial coin state when \(|\theta|\) increases. Obviously, the DTQWs defined by these generalized Grover coins localize at the vertex \((0,0)\) of the infinite lattice.
Figure 3: Numerical values of $T^\infty(\psi_S)$, $S \in \{R, L, U, D\}$ when the coins belong to $(P(23)Z_1)_\theta$ for 400 equidistant values of $\theta$ in $(-\pi, \pi)$.

3.3 With non-Grover coins

In this section, we consider the DTQWs corresponding to the coin operators which lie in $\mathcal{X}_3$, where

$$\mathcal{X}_3 = \left\{ \begin{bmatrix} x & 1-x & z & -z \\ 1-x & x & -z & z \\ z & -z & 1-x & x \\ -z & z & x & 1-x \end{bmatrix} : x^2 + z^2 - x = 0, 0 \leq x \leq 1 \right\}$$

described in Corollary 2.5. Then a one-parameter representations of elements in $(\mathcal{X}_3)_\theta$ can be obtained by setting $x = \frac{1}{2}(1 + \cos \theta)$, $-\pi \leq \theta \leq \pi$. Observe that orthogonal matrices in $\mathcal{X}_3$ are linear sum of permutations and the Grover matrix does not belong to this set. Now

$$U''_{n,m} = D_{n,m}C = \begin{bmatrix} \frac{1}{2}(1 + \cos \theta)\omega^{-n} & \frac{1}{2}(1 - \cos \theta)\omega^{-n} & \frac{1}{2}\sin \theta\omega^{-n} & -\frac{1}{2}\sin \theta\omega^{-n} \\ \frac{1}{2}\sin \theta\omega^{-m} & \frac{1}{2}(1 + \cos \theta)\omega^{-m} & -\frac{1}{2}\sin \theta\omega^{-m} & \frac{1}{2}\sin \theta\omega^{-m} \\ -\frac{1}{2}\sin \theta\omega^{m} & \frac{1}{2}(1 - \cos \theta)\omega^{m} & \frac{1}{2}\sin \theta\omega^{m} & \frac{1}{2}(1 + \cos \theta)\omega^{m} \\ \frac{1}{2}(1 - \cos \theta)\omega^{m} & -\frac{1}{2}\sin \theta\omega^{m} & \frac{1}{2}\sin \theta\omega^{m} & \frac{1}{2}(1 + \cos \theta)\omega^{m} \end{bmatrix}$$

for $-\pi \leq \theta \leq \pi$, $\omega = e^{2\pi i/N}$, $m, n \in \{0, \ldots, N - 1\}$. Now we determine a set of eigenpairs of $U''_{n,m}$ in the following lemma.

**Lemma 3.9.** The eigenvalues $\lambda_{n,m,k}$ of $U''_{n,m}$ are given as follows.

$$\lambda_{n,m,1} = -1, \lambda_{n,m,2} = 1, \lambda_{n,m,3} = e^{i\eta}, \lambda_{n,m,4} = e^{-i\eta},$$

where $\cos \eta = \frac{(1 + \cos \theta) \cos \zeta_m + (1 - \cos \theta) \cos \zeta_m - 1}{2}$ and the eigenvector corresponding to $\lambda_{n,m,k}$ is

$$v_{n,m,k} = \begin{bmatrix} -\frac{\sin \theta(1 - \lambda_{n,m,k}\omega^m)}{(1 + \cos \theta)(1 - \lambda_{n,m,k}\omega^{-n})} & \frac{\sin \theta(1 - \lambda_{n,m,k}\omega^m)}{(1 + \cos \theta)(1 - \lambda_{n,m,k}\omega^{-n})} & 1 & -\frac{1 - \lambda_{n,m,k}\omega^m}{1 - \lambda_{n,m,k}\omega^{-n}} \end{bmatrix}^T$$

for $k \in \{1, 2, 3, 4\}$ and $\zeta_q = 2\pi q/N$, $q \in \{n, m\}$.

**Proof:** The characteristic polynomial of $U''_{n,m}$ is

$$\chi_{U''_{n,m}}(\lambda) = \lambda^4 - (\cos \zeta_m + \cos \zeta_n + \cos \eta \cos \theta - \cos \zeta_m \cos \theta)\lambda^3 + (\cos \zeta_m + \cos \zeta_n + \cos \eta \cos \theta - \cos \zeta_m \cos \theta)\lambda^2 - 1.$$
Solving $\chi_{U'_{n,m}}(\lambda) = 0$ we get the required eigenvalues. □

Adapting similar procedures as in the above subsections, the values of total time-averaged probabilities $P_\infty(\psi_S), S \in \{R, L, U, D\}$ can be determined numerically for canonical initial coin states for infinite lattice. In Figure 4, we plot $P_\infty(\psi_S)$ for different values of $\theta$ obtained by discretizing the interval $(-\pi, \pi)$ into 400 equidistant points. Then observe that the total probabilities are symmetric about the vertical axis through $\theta = 0$, where it becomes zero for initial coin state $|\psi_S\rangle, S \in \{R, L\}$. Indeed, $P_\infty(\psi_S)$ increases and decreases as $|\theta|$ increases for $S \in \{U, D\}$ and $S \in \{R, L\}$, respectively. Besides, observe that the total probabilities $P_\infty(\psi_S), S \in \{U, D\}$ approach to zero for several coins when $|\theta|$ approaches to $\pi$, and $P_\infty(\psi_S) = 0$ if $\theta = 0$, which corresponds to a permutation coin when $S \in \{R, L\}$.

Figure 4: Numerical values of $P_\infty(\psi_S), S \in \{R, L, U, D\}$ when the coins belong to $(X_3)_\theta$ for 400 equidistant values of $\theta$ in $(-\pi, \pi)$.

**Conclusion.** In this paper, we have proposed discrete-time coined quantum walks (DTQWs) on two-dimensional lattices by considering the coins as (real) permutative orthogonal matrices of order $4 \times 4$. First, we have derived parametric representations of all complex, real and rational matrices of order $4 \times 4$ that are permutative orthogonal matrices. We also have attempted to characterize orthogonal matrices of order $4 \times 4$ that can be expressed as linear sum of permutation matrices. Indeed, we have identified several matrix spaces such that any orthogonal matrix in these spaces is always permutative or direct sum of permutative matrices up to permutation of its rows and columns or neither of these forms.

Based on the parametric representation of real permutative orthogonal matrices, we identify classes of matrices that contain Grover matrix as an element in those classes, which we call generalized Grover matrices or coins. We have shown that DTQWs with canonical initial coin states exhibit localization phenomena at the initial position $(0,0)$ of the infinite lattice by considering the coins as generalized Grover matrices. Finally, we have shown that the localization property of DTQWs at initial position of the walker on the infinite lattice corresponding to generalized Grover coins need not extend to DTQWs corresponding to all permutative orthogonal matrices.

**Acknowledgement.** Amrita Mandal thanks Council for Scientific and Industrial Research (CSIR), India for financial support in the form of a junior/senior research fellowship. Rohit Sarma Sarkar acknowledges support through Prime Minister Research Fellowship (PMRF), Government of India.
References

[1] Aharonov, D., Ambainis, A., Kempe, J., Vazirani, U., Quantum walks on graphs, Proceedings of the thirty-third annual ACM symposium on Theory of computing, 50–59 (2001).

[2] Ambainis, A., Kempe, J., Rivosh, A., Coins make quantum walks faster, arXiv preprint quant-ph/0402107 (2004).

[3] Brualdi, R. A., Ryser, Herbert J., Combinatorial matrix theory, Springer 39 (1991).

[4] Childs, A.M., Universal computation by quantum walk, Physical Review Letters 102, no. 18, 180501 (2009).

[5] Childs, A.M., Gosset, D., Webb, Z., Universal computation by multiparticle quantum walk, Science 339, no. 6121, 791-794 (2013).

[6] Côté, R., Russell, A., Eyler, Edward E., Gould, Phillip L., Quantum random walk with Rydberg atoms in an optical lattice, New Journal of Physics 8, no. 8, 156 (2006).

[7] D’Errico, A., Cardano, F., Maffei, M., Dauphin, A., Barboza, R., Esposito, C., Piccirillo, B., Lewenstein, M., Massignan, P., Marrucci, L., Two-dimensional topological quantum walks in the momentum space of structured light, Optica 7, no. 2, 108–114 (2020).

[8] Farahat, H.K., Sets of linearly independent permutation matrices, Journal of the London Mathematical Society 2, no. part 4, 696-698 (1970).

[9] Grover, L.K., A fast quantum mechanical algorithm for database search, Proceedings of the twenty-eighth annual ACM symposium on Theory of computing, 212-219 (1996).

[10] Inui, N., Konishi, Y., Konno, N., Localization of two-dimensional quantum walks, Physical Review A 69, no. 5, 052323 (2004).

[11] Inui, N., Konno, N., Segawa, E., One-dimensional three-state quantum walk, Physical Review E 72, no. 5, 056112 (2005).

[12] Kapoor, J., Orthogonal matrices as linear combinations of permutation matrices, Linear Algebra and its Applications 12, no. 3, 189–196 (1975).

[13] Klappenecker, A., Roetteler, M., Quantum software reusability, International Journal of Foundations of Computer Science 14, no. 05, 777-796 (2003).

[14] Kollár, B., Kiss T., Jex, I., Strongly trapped two-dimensional quantum walks, Physical Review A 91, no. 2, 022308 (2015).

[15] Konno, N., Localization of an inhomogeneous discrete-time quantum walk on the line, Quantum Information Processing 9, 405–418 (2010).

[16] Lovett, N.B., Cooper, S., Everitt, M., Trevers, M., Kendon, V., Universal quantum computation using the discrete-time quantum walk, Physical Review A 81, no. 4, 042330 (2010).

[17] Lyu, C., Yu, L., Wu, S., Localization in quantum walks on a honeycomb network, Physical Review A 92, no. 5, 052305 (2015).

[18] Mackay, T.D., Bartlett, S.D., Stephenson, L.T., Sanders, B.C., Quantum walks in higher dimensions, Journal of Physics A: Mathematical and General 35, no. 12, 2745 (2002).

[19] Mandal A., Adhikari B., Kannan, M.R., On the eigenvalue region of permutative doubly stochastic matrices, arXiv preprint arXiv:1910.01829v3, (2019).
[20] Paparella, P., Realizing Suleimanova spectra via permutative matrices, *The Electronic Journal of Linear Algebra* 31, 306–312 (2016).

[21] Peruzzo, A., Lobino, M., Matthews, J. C., Matsuda, N., Politi, A., Poulios, K., Zhou, X.Q., Lahini, Y., Ismail, N., Wörhoff, K., Bromberg, Y., Quantum walks of correlated photons, *Science* 329, no. 5998, pp.1500-1503 (2010).

[22] Sarma Sarkar, R., Mandal, A., Adhikari, B., Periodicity of lively quantum walks on cycles with generalized Grover coin, *Linear Algebra and its Applications* 604, 399–424 (2020).

[23] Schreiber, A., Gábris, A., Rohde, P.P., Laiho, K., Štefaňák, M., Potoček, V., Hamilton, C., Jex, I, Silberhorn, C., A 2D quantum walk simulation of two-particle dynamics, *Science*, 336, no. 6077, 55-58 (2012).

[24] Severini, S., Szőlősi, F., A further look into combinatorial orthogonality, *Electron. J. Linear Algebra* 17, 376–388 (2008).

[25] Štefaňák, M., Bezděková, I., Jex, I., Continuous deformations of the Grover walk preserving localization, *The European Physical Journal D* 66, no. 5, 142 (2012).

[26] Štefaňák, M., Bezděková, I., Jex, I., Limit distributions of three-state quantum walks: the role of coin eigenstates, *Physical Review A* 90, no. 1, 012342 (2014).

[27] Svozilik, J., León-Montiel, R.D.J., Torres, J.P., Implementation of a spatial two-dimensional quantum random walk with tunable decoherence, *Physical Review A* 86, no. 5, 052327 (2012).

[28] Tang, H., Lin, X.F., Feng, Z., Chen, J.Y., Gao, J., Sun, K., Wang, C.Y., Lai, P.C., Xu, X.Y., Wang, Y. and Qiao, L.F., Experimental two-dimensional quantum walk on a photonic chip, *Science advances* 4, no. 5, eaat3174 (2018).

[29] Tregenna, B., Flanagan, W., Maile, R., Kendon, V., Controlling discrete quantum walks: coins and initial states, *New Journal of Physics* 5, no. 1, 83 (2003).

[30] Venegas A., Salvador E., Quantum walks: a comprehensive review, *Quantum Information Processing* 11, no. 5, 1015-1106 (2012).

[31] Watabe, K., Kobayashi, N., Katori, M., Konno, N., Limit distributions of two-dimensional quantum walks, *Physical Review A* 77, no. 6, 062331 (2008).

[32] Wojcik, A., Luczak, T., Kurzyński, P., Grużka, A., Gdala, T., Bednarska-Bzdęga, M., Trapping a particle of a quantum walk on the line, *Physical Review A* 85, no. 1, 012329 (2012).

[33] Zeng, M., Yong, Ee, H., Discrete-time quantum walk with phase disorder: localization and entanglement entropy, *Scientific reports* 7, no. 1, 1-9 (2017).