Investigation Fermionic Quantum Walk for Detecting Nonisomorph Cospectral Graphs

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Abstract: The graph isomorphism (GI) is investigated in some cospectral networks. Two graphs are isomorphic when they are related to each other by a relabeling of the graph vertices. The GI in two scalable (n+2)-regular graphs $G_4(n;n+2)$ and $G_5(n;n+2)$, is studied analytically by using the multiparticle quantum walk. These two graphs are a pair of non-isomorphic connected cospectral regular graphs for any positive integer n. In order to investigation GI in these two graphs, the adjacency matrices of graphs have been rewritten in the antisymmetric fermionic basis. These fermionic basis are in a form that the adjacency matrices in these basis will be 8×8 for all amounts of n. Then it is shown that the multiparticle quantum walk is able to distinguish pairs of non-isomorph graphs. Rewriting the adjacency matrices of graphs in these basis reduces the complexity of calculations. Also we construct two new graphs $T_4(n;n+2)$ and $T_5(n;n+2)$ and repeat the same process of G_4 and G_5 to study the GI problem by using multiparticle quantum walk. Finally the GI has been discussed in some examples of cospectral graphs.

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1 Introduction

One of the important problems about networks is the graph isomorphism (GI) problem [1]. Two graphs are isomorphic, if one can be transformed into the other by a relabeling of vertices (i.e. , if two graphs with the same number of vertices and edges, can not be transformed into each other by relabeling of vertices, then they will be non-isomorph).

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Classical algorithm which runs in a time polynomial in the number of vertices of the graphs, is able to distinguish many graph pairs, but some pairs are distinguished computationally difficult. Currently, the best general classical algorithm has a run time $O(c^{\sqrt{N}\log N})$, where c is a constant and N is the number of vertices in the two graphs. Typical instances of graph isomorphism (GI) can be solved in polynomial time because two randomly chosen graphs with identical numbers of vertices and edges typically have different degree and eigenvalue distributions. Moreover, GI is solved efficiently for a few classes of graphs, such as trees[2], planar graphs[3], graphs with bounded degree[4], bounded eigenvalue multiplicity[5], and bounded average genus[6]. Researchers have also recently solved GI using various methods by using physical systems. Rudolph mapped the GI problem onto a system of hard-core atoms [7]. Gudkov and Nussinov proposed a physically motivated classical algorithm to distinguish non-isomorphic graphs [8].

One of the useful tools in detecting non-isomorphic graphs is quantum walk (QW). Many researchers are interested in the field of quantum walks (QWs) [9-12] which it can be implemented experimentally on a circles with single photon [13]. This interesting field has many applications in other quantum processes such as quantum search [14], quantum algorithm [15] and measuring network vertex centrality [16]. Quantum random walks (QRW)s [17-19] is the Markov process in which, at every time step, a particle moves to one of the neighboring sites as a result of the random outcome of a coin toss. Two references [20,21] are about open quantum random walks and the reference [22] is the continuous time two particle quantum walk on a one-dimensional noisy lattice. Some researchers used quantum random walks to investigate the capability of quantum walks to distinguish nonisomorphic graphs. Shiau et al. proved that the simplest classical algorithm fails to distinguish some pairs of nonisomorphic graphs and also proved that continuous-time one-particle QRWs cannot distinguish some non-isomorphic graphs [23]. Douglas and Wang modified a single-particle QRW by adding phase inhomogeneities, altering the evolution as the particle walked through the graph [24]. Emms et al. used discrete-time QRWs to build potential graph invariants [25,26]. Berry et al. studied discrete-time quantum walks on the line and on general undirected graphs with two interacting or noninteracting particles [27]. For strongly regular graphs, they showed that noninteracting discrete-time quantum walks can distinguish some but not all non-isomorph graphs with the same family parameters. Gamble et al. extended these results, proving that QRWs of two noninteracting particles will always fail to distinguish pairs of nonisomorphic SRGs with the same family parameters [28]. Then Rudinger et al. numerically demonstrated that three-particle noninteracting walks have distinguishing power on pairs of SRGs [29,30]. In [31] the authors proposed a new algorithm based on a quantum walk search model to distinguish strongly similar graphs. In our previous paper [32] we investigated GI problem in strongly regular (SRG) graphs by using the entanglement entropy. We obtained the adjacency matrix of SRG in the stratification basis, then we calculated the entanglement entropy in non-isomorph SRGs and showed that the entanglement entropy can distinguish the non-isomorph pairs of SRGs.

In this paper we use quantum walk to distinguish non-isomorph cospectral graphs.

Cospectral graphs are graphs that share the same graph spectrum. The non-isomorph cospectral scalable pairs $G_4(n, n+2)$ and $G_5(n, n+2)$ are introduced in [33]. We use n-particle quantum walk for GI problem in these graphs. to this aim we rewrite the adjacency matrices of these two graphs in the new basis. The new basis are obtained by fermionization of n-particle standard basis. The adjacency matrices of these graphs in the new basis is 8×8. So the dimension of adjacency matrices reduces to 8×8 from $(8n+12) \times (8n+12)$. Therefore the complexity of calculations reduces significantly by using this n-particle quantum walk. We give the amplitudes of n-particle quantum walk on these graphs and show that it has the ability to distinguish these non-isomorph pairs. Also we use the adjacency matrices of G_4 and G_5 to construct two new graphs which we call $T_4(n, n+2)$ and $T_5(n, n+2)$. These two graphs are Cospectral and non-isomorph for any positive integer n. We use the antisymmetric fermionic basis again and rewrite the adjacency matrices of two new graphs in these basis. By repeating the previous method for T_4 and T_5, from the difference between the amplitudes of n-particle qauntum walk, one can conclude that they are non-isomorph .

The paper is structured as follows. In Section 2 we give some preliminaries in four subsections. First we explain some interpretation about the graph and the stratification techniques in 2.1. Then in 2.2 we briefly clarify quantum walk. In section 3, first we introduce two non-isomorph graphs $G_4(n, n+2)$ and $G_5(n, n+2)$ and prove that they are cospectral. Then in 3.1 we investigate GI in these two graphs by using quantum walk in fermionic basis. The results show that the n-particle quantum walk has power of distinguishing pairs of non-isomorph graphs $G_4(n, n+2)$ and $G_5(n, n+2)$. In 3.1.1 we do the same process for two new non-isomorph graphs $T_4(n, n+2)$ and $T_5(n, n+2)$. In section 4 we give some examples of non-isomorph cospectral graphs which are distinguished by using single particle quantum walk. We discuss our conclusions in Section 5.

2 Preliminaries

2.1 Graphs and their Stratification techniques

A graph is a pair $G = (V, E)$, where V is a non-empty set and E is a subset of $\{(i, j); i, j \in V, i \neq j\}$. Elements of V and of E are called vertices and edges, respectively. Two vertices $i, j \in V$ are called adjacent if $(i, j) \in E$, and in that case we write $i \sim j$. A finite sequence $i_0; i_1; ...; i_n \in V$ is called a walk of length n (or of n steps) if $i_{k-1} \sim i_k$ for all $k = 1, 2, ..., n$. A graph is called connected if any pair of distinct vertices is connected by a walk. The degree or valency of a vertex $x \in V$ is defined by $\kappa(x) = |y \in V : y \sim x|$. The graph structure is fully represented by the adjacency matrix A defined by

$$(A)_{ij} = \begin{cases} 1 & i \sim j \\ 0 & otherwise \end{cases} \tag{1}$$

Obviously, (i) A is symmetric; (ii) an element of A takes a value in $0, 1$; (iii) a diagonal element of A vanishes. Let $l_2(V)$ denote the Hilbert space of square-summable functions on V , and $|i\rangle; i \in V$ becomes a complete orthonormal basis of $l_2(V)$. The adjacency matrix is considered as an operator acting in $l_2(V)$ in such a way that

$$A|i\rangle = \sum_{j\sim i} |j\rangle \qquad i \in V. \tag{2}$$

For $i \neq j$ let $\partial(i, j)$ be the length of the shortest walk connecting i and j. By definition $\partial(i, i) = 0$ for all $i \in V$. The graph becomes a metric space with the distance function ∂. Note that $\partial(i, j) = 1$ if and only if $i \sim j$. We fix a point $o \in V$ as an origin of the graph. Then, a natural stratification for the graph is introduced as:

$$V = \bigcup_{i=0}^{\infty} V_i(o) \qquad V_i(o) := \{j \in V : \partial(o, j) = i\} \tag{3}$$

If $V_k(o) = \emptyset$ happens for some $k \geq 1$, then $V_l(o) = \emptyset$ for all $l \geq k$. With each stratum V_i, we associate a unit vector in $l_2(V)$ defined by

$$|\phi_i\rangle = \frac{1}{\sqrt{\kappa_i}} \sum_{k\in V_i(o)} |k\rangle \tag{4}$$

where, $\kappa_i := |V_i(o)|$ and $|k\rangle$ denotes the eigenket of k-th vertex at the stratum i. The closed subspace of $l_2(V)$ spanned by $|\phi_i\rangle$ is denoted by $\Gamma(G)$. Since $|\phi_i\rangle$ becomes a complete orthonormal basis of $\Gamma(G)$, we often write

$$\Gamma(G) = \sum_k \oplus C|\phi_k\rangle \tag{5}$$

In this stratification for any connected graph G, we have

$$V_1(\beta) \subseteq V_{i-1}(\alpha) \bigcup V_i(\alpha) \bigcup V_{i+1}(\alpha) \tag{6}$$

for each $\beta \in V_i(\alpha)$. Now, recall that the i-th adjacency matrix of a graph $G = (V, E)$ is defined as

$$(A_i)_{\alpha,\beta} = \begin{cases} 1 & if \quad \partial(\alpha, \beta) = i \\ 0 & otherwise \end{cases} \tag{7}$$

Then, for reference state $|\phi_0\rangle$ ($|\phi_0\rangle = |o\rangle$), with $o \in V$ as reference vertex), we have

$$A_i|\phi_0\rangle = \sum_{\beta\in V_i(o)} |\beta\rangle. \tag{8}$$

Then by using (4) and (10), we have

$$A_i|\phi_0\rangle = \sqrt{\kappa_i}|\phi_i\rangle. \tag{9}$$

Then, for reference state $|\phi_0\rangle$ ($|\phi_0\rangle = |o\rangle$), with $o \in V$ as reference vertex), we have

$$A_i|\phi_0\rangle = \sum_{\beta \in V_i(o)} |\beta\rangle. \tag{10}$$

Then by using (4) and (10), we have

$$A_i|\phi_0\rangle = \sqrt{\kappa_i}|\phi_i\rangle. \tag{11}$$

For more details you can see [34-36].

2.2 Continuous time quantum walk

The continuous-time quantum walk is defined by replacing Kolmogorovs equation with Schrodingers equation. Let $|\phi_i(t)\rangle$ be a time-dependent amplitude of the quantum process on graph Γ. The wave evolution of the quantum walk is

$$i\hbar\frac{d}{dt}|\phi(t)\rangle = H|\phi(t)\rangle \tag{12}$$

where we assume $\hbar = 1$ and $|\phi_0\rangle$ is the initial amplitude wave function of the particle. The solution is given by

$$|\phi_0(t)\rangle = e^{-iHt}|\phi_0\rangle \tag{13}$$

Where elements of amplitudes between strata are calculated

$$\langle\phi_i(t)|\phi_0(t)\rangle = \langle\phi_i(t)|e^{-iHt}|\phi_0\rangle \tag{14}$$

Obviously the above result indicates that the amplitudes of observing walk on vertices belonging to a given stratum are the same. Actually one can straightforwardly the transition probabilities between the vertices depend only on the distance between the vertices irrespective of which site the walk has started. So, if stratification of two non-isomorphism graph is different, the quantum walk on these graphs are different.

3 Investigation of graph isomorphism (GI) problem in $G_4(n, n+2)$ and $G_5(n, n+2)$

In this section, the graphs $G_4(n, n+2)$ and $G_5(n, n+2)$ with $8n+12$ vertices are defined. The $(n+2)$-regular graphs $G_4(n, n+2)$ and $G_5(n, n+2)$ are a pair of connected cospectral integral regular graphs for any positive integer n. We prove that these two graphs are non isomorphic by using the fermionic quantum walk. The adjacency of $G_4(n, n+2)$ are defined as

$$A(G_4(n, n+2)) = \begin{pmatrix} A_0 & A_1 \\ A_1 & A_0 \end{pmatrix} \tag{15}$$

where

$$A_0(G_4) = \begin{pmatrix} 0 & J_{n\times(n+2)} & 0 & 0 \\ J_{(n+2)\times n} & 0 & I_{(n+2)} & 0 \\ 0 & I_{(n+2)} & 0 & B_{(n+2)} \\ 0 & 0 & B_{(n+2)} & 0 \end{pmatrix} \tag{16}$$

and

$$A_1(G_4) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & I_{(n+2)} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I_{(n+2)} \end{pmatrix} \tag{17}$$

and

$$B = \begin{pmatrix} 1 & J_{1,n} & 0 \\ J_{n,1} & J_n - I_n & J_{n,1} \\ 0 & J_{1,n} & 1 \end{pmatrix} \tag{18}$$

After some relabeling, the total adjacency matrix for $G_4(n, n+2)$ is

$$A(G_4(a,b)) = \begin{pmatrix} 0 & 0 & J_{n\times(n+2)} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & I_{(n+2)} & B_{(n+2)} & 0 & 0 & 0 & 0 \\ J_{(n+2)\times n} & I_{(n+2)} & 0 & 0 & I_{(n+2)} & 0 & 0 & 0 \\ 0 & B_{(n+2)} & 0 & 0 & 0 & I_{(n+2)} & 0 & 0 \\ 0 & 0 & I_{(n+2)} & 0 & 0 & 0 & J_{(n+2)\times n} & I_{(n+2)} \\ 0 & 0 & 0 & I_{(n+2)} & 0 & 0 & 0 & B_{(n+2)} \\ 0 & 0 & 0 & 0 & J_{n\times(n+2)} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & I_{(n+2)} & B_{(n+2)} & 0 & 0 \end{pmatrix} \tag{19}$$

The adjacency matrix for $G_5(n, n+2)$ is

$$A(G_5(a,b)) = \begin{pmatrix} A_0 & A_1 \\ A_1 & A_0 \end{pmatrix} \tag{20}$$

where A_0 and A_1 for $G_5(n, n+2)$ are

$$A_0(G_5) = \begin{pmatrix} 0 & J_{n\times(n+2)} & 0 & 0 \\ J_{(n+2)\times n} & 0 & I_{(n+2)} & I_{(n+2)} \\ 0 & I_{(n+2)} & 0 & 0 \\ 0 & I_{(n+2)} & 0 & 0 \end{pmatrix} \tag{21}$$

and

$$A_1(G_5) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & B_{(n+2)} & 0 \\ 0 & 0 & 0 & B_{(n+2)} \end{pmatrix} \tag{22}$$

and the matrix B is the same as the $G_4(n, n+2)$. After some relabeling, the adjacency matrix of $G_5(n, n+2)$ is

$$A(G_5(a,b)) = \begin{pmatrix} 0 & J_{n\times(n+2)} & 0 & 0 & 0 & 0 & 0 & 0 \\ J_{(n+2)\times n} & 0 & I_{(n+2)} & I_{(n+2)} & 0 & 0 & 0 & 0 \\ 0 & I_{(n+2)} & 0 & 0 & B_{(n+2)} & 0 & 0 & 0 \\ 0 & I_{(n+2)} & 0 & 0 & 0 & B_{(n+2)} & 0 & 0 \\ 0 & 0 & B_{(n+2)} & 0 & 0 & 0 & I_{(n+2)} & 0 \\ 0 & 0 & 0 & B_{(n+2)} & 0 & 0 & I_{(n+2)} & 0 \\ 0 & 0 & 0 & 0 & I_{(n+2)} & I_{(n+2)} & 0 & J_{(n+2)\times n} \\ 0 & 0 & 0 & 0 & 0 & 0 & J_{n\times(n+2)} & 0 \end{pmatrix} \tag{23}$$

Now we want to show that two graphs $G_4(n, n+2)$ and $G_5(n, n+2)$ are Cospectral. The adjacency matrices of these graphs can be written as

$$A = I_2 \otimes A_0 + \sigma_x \otimes A_1$$

So the eigenvalues of adjacency matrices of these two graphs will be the eigenvalues of two matrices $A_0 \pm A_1$.

$$(A_0 \pm A_1)(G_4) = \begin{pmatrix} 0 & J_{n\times(n+2)} & 0 & 0 \\ J_{(n+2)\times n} & \pm I_{(n+2)} & I_{(n+2)} & 0 \\ 0 & I_{(n+2)} & 0 & B_{(n+2)} \\ 0 & 0 & B_{(n+2)} & \pm I_{(n+2)} \end{pmatrix} \tag{24}$$

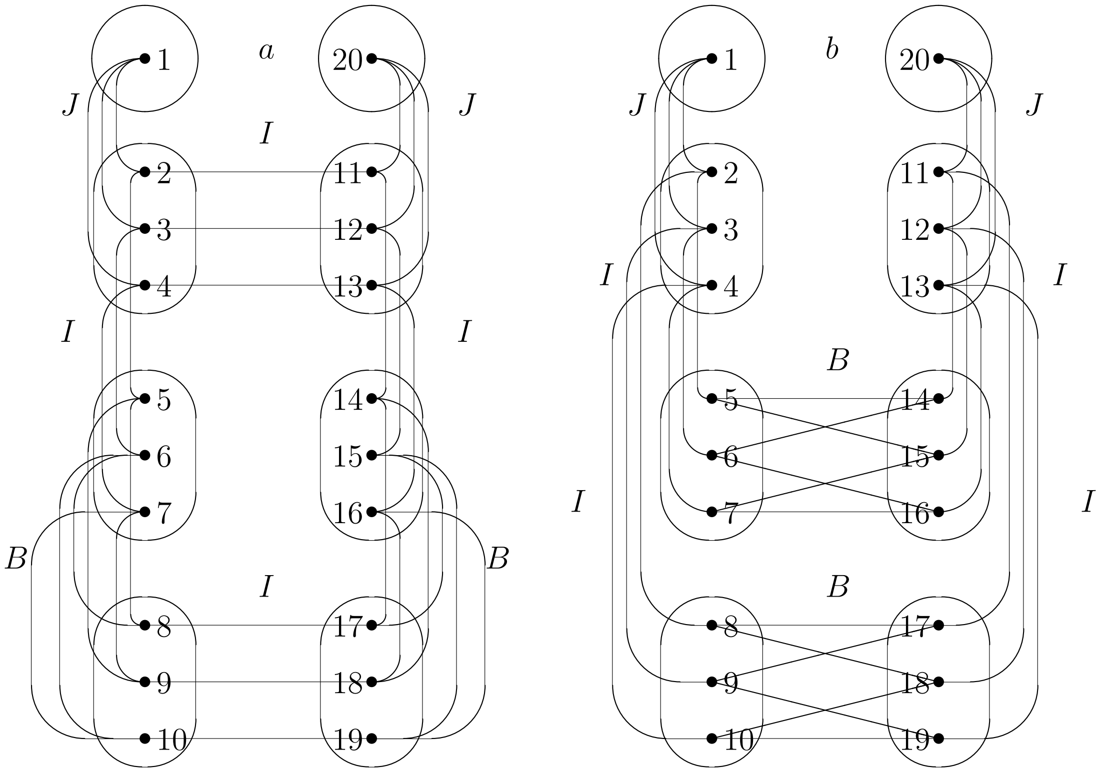

Figure 1 An example of $G_4(n, n+2)$ in (a) and $G_5(n, n+2)$ in (b) with $n = 1$.

We want to diagonalize the blocks of above matrix. So we can apply following transformation

$$= \begin{pmatrix} O_1^T & 0 & 0 & 0 \\ 0 & O_2^T & 0 & 0 \\ 0 & 0 & O_3^T & 0 \\ 0 & 0 & 0 & O_4^T \end{pmatrix} \begin{pmatrix} 0 & J_{n\times(n+2)} & 0 & 0 \\ J_{(n+2)\times n} & \pm I_{(n+2)} & I_{(n+2)} & 0 \\ 0 & I_{(n+2)} & 0 & B_{(n+2)} \\ 0 & 0 & B_{(n+2)} & \pm I_{(n+2)} \end{pmatrix} \begin{pmatrix} O_1 & 0 & 0 & 0 \\ 0 & O_2 & 0 & 0 \\ 0 & 0 & O_3 & 0 \\ 0 & 0 & 0 & O_4 \end{pmatrix} \tag{25}$$

$$= \begin{pmatrix} 0 & O_1^T J_{n\times(n+2)} O_2 & 0 & 0 \\ O_2^T J_{(n+2)\times n} O_1 & \pm O_2^T O_2 & O_2^T O_3 & 0 \\ 0 & O_3^T O_2 & 0 & O_3^T B_{(n+2)} O_4 \\ 0 & 0 & O_4^T B_{(n+2)} O_3 & \pm O_4^T O_4 \end{pmatrix}$$

Then by choosing $O_2 = O_3 = O_4$, the transformed matrix will be

$$\begin{pmatrix} 0 & SVD(J_{n\times(n+2)}) & 0 & 0 \\ SVD(J_{(n+2)\times n}) & \pm I_{(n+2)} & I_{(n+2)} & 0 \\ 0 & I_{(n+2)} & 0 & D_B \\ 0 & 0 & D_B & \pm I_{(n+2)} \end{pmatrix} \tag{26}$$

Therefore the eigenvalues of G_4 will be the eigenvalues of these matrices:

$$\begin{pmatrix} 0 & \sqrt{n(n+2)} & 0 & 0 \\ \sqrt{n(n+2)} & \pm 1 & 1 & 0 \\ 0 & 1 & 0 & n+1 \\ 0 & 0 & n+1 & \pm 1 \end{pmatrix}, \qquad \begin{pmatrix} \pm 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & \pm 1 \end{pmatrix} \tag{27}$$

The eigenvalues will be

$$\pm(n+2), \underbrace{\pm(n+1)}_{2times}, \pm n, \underbrace{\pm 2}_{(n+1)times}, \underbrace{\pm 1}_{2(n+1)times}$$

The same process can be applied to graph G_5, So the eigenvalues of adjacency matrix of graph G_5 will be the eigenvalues of these matrices:

$$\begin{pmatrix} 0 & \sqrt{n(n+2)} & 0 & 0 \\ \sqrt{n(n+2)} & 0 & 1 & 1 \\ 0 & 1 & \pm(n+1) & 0 \\ 0 & 1 & 0 & \pm(n+1) \end{pmatrix}, \qquad \begin{pmatrix} 0 & 1 & 1 \\ 1 & \pm 1 & 0 \\ 1 & 0 & \pm 1 \end{pmatrix} \tag{28}$$

The eigenvalues will be

$$\pm(n+2), \underbrace{\pm(n+1)}_{2times}, \pm n, \underbrace{\pm 2}_{(n+1)times}, \underbrace{\pm 1}_{2(n+1)times}$$

So these two graphs for all n are cospectral.

3.1 Investigation of GI problem via quantum walk in the antisymmetric fermionic basis

Now we want to use quantum walk for investigating graph isomorphism problem in these two graphs. The total adjacency matrix for $G_4(n,(n+2))$ can be written as

$$A(G_4)=\begin{pmatrix} 0 & J_{n\times(n+2)} & 0 & 0 & 0 & 0 & 0 & 0\\ J_{(n+2)\times n} & 0 & I_{(n+2)} & 0 & I_{(n+2)} & 0 & 0 & 0\\ 0 & I_{(n+2)} & 0 & B_{(n+2)} & 0 & 0 & 0 & 0\\ 0 & 0 & B_{(n+2)} & 0 & 0 & 0 & I_{(n+2)} & 0\\ 0 & I_{(n+2)} & 0 & 0 & 0 & I_{(n+2)} & 0 & J_{(n+2)\times n}\\ 0 & 0 & 0 & 0 & I_{(n+2)} & 0 & B_{(n+2)} & 0\\ 0 & 0 & 0 & I_{(n+2)} & 0 & B_{(n+2)} & 0 & 0\\ 0 & 0 & 0 & 0 & J_{n\times(n+2)} & 0 & 0 & 0 \end{pmatrix} \tag{29}$$

And the adjacency matrix of $G_5(n,n+2)$ can be written as

$$A(G_5)=\begin{pmatrix} 0 & J_{n\times(n+2)} & 0 & 0 & 0 & 0 & 0 & 0\\ J_{(n+2)\times n} & 0 & I_{(n+2)} & I_{(n+2)} & 0 & 0 & 0 & 0\\ 0 & I_{(n+2)} & 0 & 0 & 0 & B_b & 0 & 0\\ 0 & I_{(n+2)} & 0 & 0 & 0 & 0 & B_{(n+2)} & 0\\ 0 & 0 & 0 & 0 & 0 & I_{(n+2)} & I_{(n+2)} & J_{(n+2)\times n}\\ 0 & 0 & B_{(n+2)} & 0 & I_{(n+2)} & 0 & 0 & 0\\ 0 & 0 & 0 & B_{(n+2)} & I_b & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & J_{n\times(n+2)} & 0 & 0 & 0 \end{pmatrix} \tag{30}$$

We want to rewrite the adjacency matrices of these two graphs in the new basis.

The strata of $G_4(n,n+2)$ and $G_5(n,n+2)$ are obtained by fermionization as following form

$$|\phi_0\rangle=\frac{1}{\sqrt{n!}}\sum_{i_1,i_2,\dots,i_n}\varepsilon_{i_1,i_2,\dots,i_n}|i_1\rangle\otimes|i_2\rangle\otimes\ldots\otimes|i_n\rangle$$

$$|\phi_l\rangle=\frac{1}{\sqrt{n!}\sqrt{n(n+2)}}\sum_{i_1,i_2,\dots,i_n}\varepsilon_{i_1,i_2,\dots,i_n}|i_1\rangle\otimes|i_2\rangle\otimes\ldots\otimes|i_{k-1}\rangle(\sum_{j=1}^{n+2}|n+(l-1)(n+2)+j\rangle)\otimes|i_{k+1}\rangle\ldots\otimes|i_n\rangle \tag{31}$$

$$(l=1,\dots,6)$$

$$|\phi_7\rangle = \frac{1}{\sqrt{n!}} \sum_{i_1,i_2,\ldots,i_n} \varepsilon_{i_1,i_2,\ldots,i_n 1,2,\ldots,n} |n{+}6(n{+}2){+}i_1\rangle \otimes |n{+}6(n{+}2){+}i_2\rangle \otimes \ldots \otimes |n{+}6(n{+}2){+}i_n\rangle \tag{32}$$

The dimension of this fermionic space is $\begin{pmatrix} N \\ n \end{pmatrix}$ But we choose the above antisymmetric n-particle fermionic basis for graphs $G_4(n, n+2)$ and $G_5(n, n+2)$. We want to apply the following adjacency matrices of two graphs on the defined basis.

$$A = \sum_i I \otimes I \otimes \ldots \otimes \underbrace{A_1}_{i} \otimes I \ldots \otimes I \tag{33}$$

where I is identity matrix. Now, by applying adjacency matrices of $G_4(n, n+2)$ and $G_5(n, n+2)$ on the new basis, we have

$$\begin{aligned}
A_{G_4(n,n+2)}|\phi_0\rangle &= \sqrt{n(n+2)}|\phi_1\rangle \\
A_{G_4(n,n+2)}|\phi_1\rangle &= \sqrt{n(n+2)}|\phi_0\rangle + |\phi_2\rangle + |\phi_4\rangle \\
A_{G_4(n,n+2)}|\phi_2\rangle &= |\phi_1\rangle + (n+1)|\phi_3\rangle \\
A_{G_4(n,n+2)}|\phi_3\rangle &= (n+1)|\phi_2\rangle + |\phi_6\rangle \\
A_{G_4(n,n+2)}|\phi_4\rangle &= \sqrt{n(n+2)}|\phi_7\rangle \\
A_{G_4(n,n+2)}|\phi_5\rangle &= (n+1)|\phi_6\rangle + |\phi_4\rangle \\
A_{G_4(n,n+2)}|\phi_6\rangle &= |\phi_3\rangle + (n+1)|\phi_5\rangle \\
A_{G_4(n,n+2)}|\phi_7\rangle &= \sqrt{n(n+2)}|\phi_4\rangle
\end{aligned} \tag{34}$$

So, the adjacency matrix in the stratification basis is

$$A_{G_4(n,n+2)} = \begin{pmatrix}
0 & \sqrt{n(n+2)} & 0 & 0 & 0 & 0 & 0 & 0 \\
\sqrt{n(n+2)} & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & n+1 & 0 & 0 & 0 & 0 \\
0 & 0 & n+1 & 0 & 0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & \sqrt{n(n+2)} \\
0 & 0 & 0 & 0 & 1 & 0 & n+1 & 0 \\
0 & 0 & 0 & 1 & 0 & n+1 & 0 & 0 \\
0 & 0 & 0 & 0 & \sqrt{n(n+2)} & 0 & 0 & 0
\end{pmatrix} \tag{35}$$

The amplitudes of quantum walk (i.e. $\langle\phi_i|e^{-iHt}|\phi_0\rangle = \langle\phi_i|e^{-iA_{G_4}t}|\phi_0\rangle$) for G_4 are

$$\langle\phi_0|e^{-iA_{G_4}t}|\phi_0\rangle =$$

$$\frac{n^2+2n}{2(n+1)^2}\cos(n+1)t + \frac{n^2}{2(2n^2+3n)}\cos(n+2)t + \frac{n^2+2n}{4n^2+2n}\cos nt$$

$$\langle\phi_1|e^{-iA_{G_4}t}|\phi_0\rangle =$$

$$-i\frac{\sqrt{n^2+2n}}{2(n+1)}\sin(n+1)t - i\frac{n\sqrt{n^2+2n}}{2(2n^2+3n)}\sin(n+2)t - i\frac{n\sqrt{n^2+2n}}{4n^2+2n}\sin nt$$

$$\langle\phi_2|e^{-iA_{G_4}t}|\phi_0\rangle =$$

$$\frac{\sqrt{n^2+2n}}{2(n+1)^2}\cos(n+1)t + \frac{n\sqrt{n^2+2n}}{2(2n^2+3n)}\cos(n+2)t + \frac{n\sqrt{n^2+2n}}{4n^2+2n}\cos nt$$

$$\langle\phi_3|e^{-iA_{G_4}t}|\phi_0\rangle = -i\frac{n\sqrt{n^2+2n}}{2(2n^2+3n)}\sin(n+2)t + i\frac{n\sqrt{n^2+2n}}{4n^2+2n}\sin nt$$

$$\langle\phi_4|e^{-iA_{G_4}t}|\phi_0\rangle = \frac{n\sqrt{n^2+2n}}{2(2n^2+3n)}\cos(n+2)t - \frac{n\sqrt{n^2+2n}}{4n^2+2n}\cos nt$$

$$\langle\phi_5|e^{-iA_{G_4}t}|\phi_0\rangle =$$

$$i\frac{\sqrt{n^2+2n}}{2(n+1)^2}\sin(n+1)t - i\frac{n\sqrt{n^2+2n}}{2(2n^2+3n)}\sin(n+2)t - i\frac{n\sqrt{n^2+2n}}{4n^2+2n}\sin nt$$

$$\langle\phi_6|e^{-iA_{G_4}t}|\phi_0\rangle =$$

$$-\frac{\sqrt{n^2+2n}}{2(n+1)^2}\cos(n+1)t + \frac{n\sqrt{n^2+2n}}{2(2n^2+3n)}\cos(n+2)t + \frac{n\sqrt{n^2+2n}}{4n^2+2n}\cos nt$$

$$\langle\phi_7|e^{-iA_{G_4}t}|\phi_0\rangle = -i\frac{n^2}{2(2n^2+3n)}\sin(n+2)t + i\frac{n^2+2n}{4n^2+2n}\sin nt$$

The effect of adjacency matrix of G_5 on the stratification basis are

$$\begin{aligned}
A_{G_5(n,n+2)}|\phi_0\rangle &= \sqrt{n(n+2)}|\phi_1\rangle \\
A_{G_5(n,n+2)}|\phi_1\rangle &= \sqrt{n(n+2)}|\phi_0\rangle + |\phi_2\rangle + |\phi_3\rangle \\
A_{G_5(n,n+2)}|\phi_2\rangle &= |\phi_1\rangle + (n+1)|\phi_5\rangle \\
A_{G_5(n,n+2)}|\phi_3\rangle &= |\phi_1\rangle + (n+1)|\phi_6\rangle \\
A_{G_5(n,n+2)}|\phi_4\rangle &= |\phi_5\rangle + |\phi_6\rangle + \sqrt{n(n+2)}|\phi_7\rangle \\
A_{G_5(n,n+2)}|\phi_5\rangle &= (n+1)|\phi_2\rangle + |\phi_4\rangle \\
A_{G_5(n,n+2)}|\phi_6\rangle &= (n+1)|\phi_3\rangle + |\phi_4\rangle \\
A_{G_5(n,n+2)}|\phi_7\rangle &= \sqrt{n(n+2)}|\phi_4\rangle
\end{aligned} \tag{36}$$

So, the adjacency matrix in the stratification basis is

$$A_{G_5(n,n+2)} = \begin{pmatrix} 0 & \sqrt{n(n+2)} & 0 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{n(n+2)} & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & n+1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & n+1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & \sqrt{n(n+2)} \\ 0 & 0 & n+1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & n+1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{n(n+2)} & 0 & 0 & 0 \end{pmatrix} \tag{37}$$

The difference between amplitudes of quantum walk for two non-isomorph graphs $G_4(n, n+2)$ and $G_5(n, n+2)$ are

$$\langle\phi_0|e^{-iA_{G_4}t}|\phi_0\rangle - \langle\phi_0|e^{-iA_{G_5}t}|\phi_0\rangle = 0$$

$$\langle\phi_1|e^{-iA_{G_4}t}|\phi_0\rangle - \langle\phi_1|e^{-iA_{G_5}t}|\phi_0\rangle = 0$$

$$\langle\phi_2|e^{-iA_{G_4}t}|\phi_0\rangle - \langle\phi_2|e^{-iA_{G_5}t}|\phi_0\rangle = 0$$

$$\langle\phi_3|e^{-iA_{G_4}t}|\phi_0\rangle - \langle\phi_3|e^{-iA_{G_5}t}|\phi_0\rangle =$$

$$\sqrt{n(n+2)}(\frac{e^{nit}}{2(2n+1)} - \frac{e^{-(n+1)it}}{(2n+1)(2n+3)} - \frac{e^{(n+2)it}}{2(2n+3)})$$

$$\langle\phi_4|e^{-iA_{G_4}t}|\phi_0\rangle - \langle\phi_4|e^{-iA_{G_5}t}|\phi_0\rangle =$$

$$\sqrt{n(n+2)}(-\frac{e^{-nit}}{2(2n+1)} - \frac{e^{nit}}{2(2n+1)} + \frac{e^{-(n+1)it}}{2(2n+1)} + \frac{e^{(n+1)it}}{2(2n+1)})$$

$$\langle\phi_5|e^{-iA_{G_4}t}|\phi_0\rangle - \langle\phi_5|e^{-iA_{G_5}t}|\phi_0\rangle =$$

$$\sqrt{n(n+2)}(\frac{e^{-nit}}{2(2n+1)} - \frac{e^{nit}}{2(2n+1)} - \frac{e^{-(n+1)it}}{2(2n+1)} + \frac{e^{(n+1)it}}{2(2n+1)})$$

$$\langle\phi_6|e^{-iA_{G_4}t}|\phi_0\rangle - \langle\phi_6|e^{-iA_{G_5}t}|\phi_0\rangle =$$

$$\sqrt{n(n+2)}(\frac{e^{-nit}}{2(2n+1)} - \frac{e^{(n+1)it}}{2(2n+3)} - \frac{e^{-(n+1)it}}{2(2n+1)} + \frac{e^{(n+2)it}}{2(2n+1)})$$

$$\langle\phi_7|e^{-iA_{G_4}t}|\phi_0\rangle - \langle\phi_7|e^{-iA_{G_5}t}|\phi_0\rangle =$$

$$(-\frac{e^{-nit}}{(n+1)} + \frac{e^{nit}}{2(2n+1)} + \frac{e^{-(n+1)it}}{(2n+1)} - \frac{e^{(n+1)it}}{(2n+1)})$$

So from the difference between the amplitudes of n-particle quantum walk, we conclude that the multiparticle quantum walk can distinguish two non-isomorph graphs. The complexity of calculations is reduced by fermionization of standard basis, and rewriting the adjacency matrices of graphs in these basis. By this method, the process of finding the amplitudes of quantum walk is done, by using the 8×8-dimensional adjacency matrix for all amount of n. But if we didn't use the new basis, then we had to work with $(8n+12) \times (8n+12)$-dimensional adjacency matrices.

3.2 Investigation of GI problem via quantum walk in $T_4(n, n+2)$ and $T_5(n, n+2)$

We can construct two nonisomorph graphs similar to $G_4(n, n+2)$ and $G_5(n, n+2)$ by replacing the A_0 and A_1 in adjacency matrices. The new graphs $T_4(n, n+2)$ and $T_5(n, n+2)$ are cospectral and non-isomorph.

$$A = \begin{pmatrix} A_1 & A_0 \\ A_0 & A_1 \end{pmatrix} \tag{38}$$

Where A_0, A_1 are the same as (16), (17) for T_4 and (21), (22) for T_5. We use the antisymmetric fermionic basis of (32) .Then, by applying adjacency matrix of $T_4(n, n+2)$ and $T_5(n, n+2)$ on these basis, we have

$$\begin{aligned}
A_{T_4(n,n+2)}|\phi_0\rangle &= \sqrt{n(n+2)}|\phi_4\rangle \\
A_{T_4(n,n+2)}|\phi_1\rangle &= \sqrt{n(n+2)}|\phi_7\rangle + |\phi_1\rangle + |\phi_5\rangle \\
A_{T_4(n,n+2)}|\phi_2\rangle &= |\phi_4\rangle + (n+1)|\phi_6\rangle \\
A_{T_4(n,n+2)}|\phi_3\rangle &= (n+1)|\phi_5\rangle + |\phi_3\rangle \\
A_{T_4(n,n+2)}|\phi_4\rangle &= \sqrt{n(n+2)}|\phi_0\rangle + |\phi_2\rangle + |\phi_4\rangle \\
A_{T_4(n,n+2)}|\phi_5\rangle &= (n+1)|\phi_3\rangle + |\phi_1\rangle \\
A_{T_4(n,n+2)}|\phi_6\rangle &= |\phi_6\rangle + (n+1)|\phi_2\rangle \\
A_{T_4(n,n+2)}|\phi_7\rangle &= \sqrt{n(n+2)}|\phi_1\rangle
\end{aligned} \tag{39}$$

So, the adjacency matrix of $T_4(n, n+2)$ in the antisymmetric fermionic basis is

$$A_{T_4(n,n+2)} = \begin{pmatrix}
0 & 0 & 0 & 0 & \sqrt{n(n+2)} & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & \sqrt{n(n+2)} \\
0 & 0 & 0 & 0 & 1 & 0 & n+1 & 0 \\
0 & 0 & 0 & 1 & 0 & n+1 & 0 & 0 \\
\sqrt{n(n+2)} & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & n+1 & 0 & 0 & 0 & 0 \\
0 & 0 & n+1 & 0 & 0 & 0 & 1 & 0 \\
0 & \sqrt{n(n+2)} & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} \tag{40}$$

And

$$A_{T_5(n,n+2)}|\phi_0\rangle = \sqrt{n(n+2)}|\phi_4\rangle$$

$$A_{T_5(n,n+2)}|\phi_1\rangle = \sqrt{n(n+2)}|\phi_7\rangle + |\phi_5\rangle + |\phi_6\rangle$$

$$A_{T_5(n,n+2)}|\phi_2\rangle = |\phi_4\rangle + (n+1)|\phi_2\rangle$$

$$A_{T_5(n,n+2)}|\phi_3\rangle = |\phi_4\rangle + (n+1)|\phi_3\rangle$$

$$A_{T_5(n,n+2)}|\phi_4\rangle = |\phi_2\rangle + |\phi_3\rangle + \sqrt{n(n+2)}|\phi_0\rangle$$

$$A_{T_5(n,n+2)}|\phi_5\rangle = (n+1)|\phi_5\rangle + |\phi_1\rangle$$

$$A_{T_5(n,n+2)}|\phi_6\rangle = (n+1)|\phi_6\rangle + |\phi_1\rangle$$

$$A_{T_5(n,n+2)}|\phi_7\rangle = \sqrt{n(n+2)}|\phi_1\rangle \tag{41}$$

So, the adjacency matrix of $T_5(n, n+2)$ in the antisymmetric fermionic basis is

$$A_{T_5(n,n+2)} = \begin{pmatrix} 0 & 0 & 0 & 0 & \sqrt{n(n+2)} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & \sqrt{n(n+2)} \\ 0 & 0 & n+1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & n+1 & 1 & 0 & 0 & 0 \\ \sqrt{n(n+2)} & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & n+1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & n+1 & 0 \\ 0 & \sqrt{n(n+2)} & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{42}$$

Non-isomorphism of two cospectral graphs can be determined by n-particle quantum walk as the same as $G_4(n, n+2)$ and $G_5(n, n+2)$ by calculating 8 amplitudes of continuous time quantum walks. Similar to $G_4(n, n+2)$ and $G_5(n, n+2)$ there is no difference between 3 amplitudes of $T_4(n, n+2)$ and $T_5(n, n+2)$. But 5 amplitudes are different. for example one of them is:

$$\langle\phi_2|e^{-iA_{T_4}t}|\phi_0\rangle - \langle\phi_2|e^{-iA_{T_5}t}|\phi_0\rangle =$$

$$\sqrt{n(n+2)}\left(\frac{1}{2(2n+1)}(e^{-nit} - e^{nit}) - \frac{1}{2(n+1)(2n+1)}(e^{-2it} - e^{2it})\right)$$

So the n-particle quantum walk is able to distinguish non-isomorph graphs.

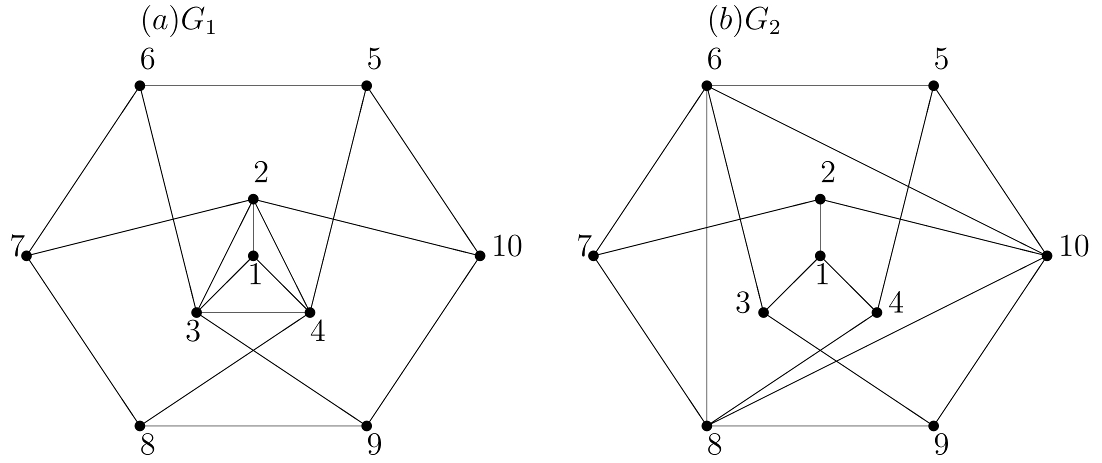

Figure 2 A pair of nonisomorphic cospectral graphs: (a) : G_1 and (b) : G_2. Single particle quantum walk can distinguish these two graphs.

4 Investigation of graph isomorphism via quantum walk in some cospectral graphs

4.1 Example I

: Two cospectral nonisomorph graphs G_1 and G_2 are shown in Fig (II). They have ten vertices and eighteen edges. The degree distribution of two graphs is $5, 5, 5, 3, 3, 3, 3, 3, 3, 3$.

The stratification basis are defined in two graph G_1 and G_2 as following

$$|\phi_0\rangle = |1\rangle$$
$$|\phi_1\rangle = \frac{1}{\sqrt{3}}(|2\rangle + |3\rangle + |4\rangle)$$
$$|\phi_2\rangle = \frac{1}{\sqrt{3}}(|5\rangle + |7\rangle + |9\rangle)$$
$$|\phi_3\rangle = \frac{1}{\sqrt{3}}(|6\rangle + |8\rangle + |10\rangle) \qquad (43)$$

So

$$A_{G_1}|\phi_0\rangle = \sqrt{3}|\phi_1\rangle$$
$$A_{G_1}|\phi_1\rangle = \sqrt{3}|\phi_0\rangle + 2|\phi_1\rangle + |\phi_2\rangle + |\phi_3\rangle$$
$$A_{G_1}|\phi_2\rangle = |\phi_1\rangle + 2|\phi_3\rangle$$
$$A_{G_1}|\phi_3\rangle = |\phi_1\rangle + 2|\phi_2\rangle \qquad (44)$$

And

$$A_{G_2}|\phi_0\rangle = \sqrt{3}|\phi_1\rangle$$

$$A_{G_2}|\phi_1\rangle = \sqrt{3}|\phi_0\rangle + |\phi_2\rangle + |\phi_3\rangle$$
$$A_{G_2}|\phi_2\rangle = |\phi_1\rangle + 2|\phi_3\rangle$$
$$A_{G_2}|\phi_3\rangle = |\phi_1\rangle + 2|\phi_2\rangle + 2|\phi_3\rangle \tag{45}$$

So, the adjacency matrix on strata basis is

$$A_{G_1} = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 2 & 1 & 1 \\ 0 & 1 & 0 & 2 \\ 0 & 1 & 2 & 0 \end{pmatrix} \tag{46}$$

$$A_{G_2} = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 1 & 1 \\ 0 & 1 & 0 & 2 \\ 0 & 1 & 2 & 2 \end{pmatrix} \tag{47}$$

$$\langle\phi_0|e^{-iA_{G_1}t} - e^{-iA_{G_2}t}|\phi_0\rangle =$$
$$-0.375e^{2it} + 0.5799e^{1.1774it} - 0.2852e^{-1.3216it} + 0.0804e^{-3.8558it}$$
$$\langle\phi_1|e^{-iA_{G_1}t} - e^{-iA_{G_2}t}|\phi_0\rangle =$$
$$0.5e^{2it} + 0.268e^{1.1774it} - 0.1661e^{-1.3216it} + 0.3981e^{-3.8558it}$$
$$\langle\phi_2|e^{-iA_{G_1}t} - e^{-iA_{G_2}t}|\phi_0\rangle =$$
$$0.375e^{2it} - 0.5799e^{1.1774it} + 0.2852e^{-1.3216it} - 0.0804e^{-3.8558it}$$
$$\langle\phi_3|e^{-iA_{G_1}t} - e^{-iA_{G_2}t}|\phi_0\rangle =$$
$$0.4999e^{2it} - 0.268e^{1.1774it} + 0.1661e^{-1.3216it} - 0.3981e^{-3.8558it}$$

We see that there are difference between the amplitudes of single particle quantum walk. then graph isomorphism can be distinguished from the single particle quantum walk.

4.2 Example II:

Two cospectral nonisomorph graphs H_1 and H_2 are shown in Fig (3). They have 12 vertices and 33 edges. The degree distribution of two graphs are

$$8, 8, 8, 8, 8, 8, 3, 3, 3, 3, 3, 3$$

The stratification basis are defined in the graph H_1 as following

$$|\phi_0\rangle = |6\rangle$$

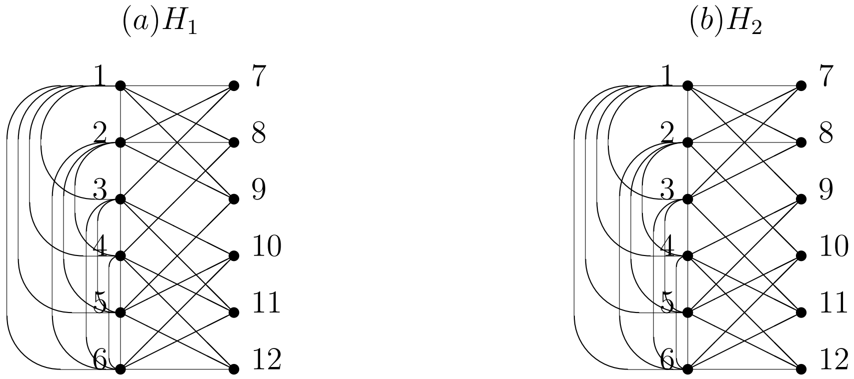

Figure 3 A pair of nonisomorphic cospectral graphs:(a) : H_1 in the left and the (b) : H_2 in the right. Single particle quantum walk can distinguish these two graphs.

$$
\begin{aligned}
|\phi_1\rangle &= \frac{1}{\sqrt{3}}(|10\rangle + |11\rangle + |12\rangle)\\
|\phi_2\rangle &= \frac{1}{\sqrt{3}}(|3\rangle + |4\rangle + |5\rangle)\\
|\phi_3\rangle &= \frac{1}{\sqrt{3}}(|7\rangle + |8\rangle + |9\rangle)\\
|\phi_4\rangle &= \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)
\end{aligned} \tag{48}
$$

So

$$
\begin{aligned}
A_{H_1}|\phi_0\rangle &= \sqrt{3}|\phi_1\rangle + \sqrt{2}|\phi_4\rangle + \sqrt{3}|\phi_2\rangle\\
A_{H_1}|\phi_1\rangle &= \sqrt{3}|\phi_0\rangle + 2|\phi_2\rangle\\
A_{H_1}|\phi_2\rangle &= \sqrt{3}|\phi_0\rangle + 2|\phi_1\rangle + 2|\phi_2\rangle + |\phi_3\rangle + \sqrt{6}|\phi_4\rangle\\
A_{H_1}|\phi_3\rangle &= \sqrt{6}|\phi_4\rangle + |\phi_2\rangle\\
A_{H_1}|\phi_4\rangle &= \sqrt{2}|\phi_0\rangle + \sqrt{6}|\phi_2\rangle + \sqrt{6}|\phi_3\rangle + |\phi_4\rangle
\end{aligned} \tag{49}
$$

$$
A_{H_1} = \begin{pmatrix} 0 & \sqrt{3} & \sqrt{3} & 0 & \sqrt{2} \\ \sqrt{3} & 0 & 2 & 0 & 0 \\ \sqrt{3} & 2 & 2 & 1 & \sqrt{6} \\ 0 & 0 & 1 & 0 & \sqrt{6} \\ \sqrt{2} & 0 & \sqrt{6} & \sqrt{6} & 1 \end{pmatrix} \tag{50}
$$

The stratification basis are defined in the graph H_2 as following

$$
|\phi_0\rangle = |12\rangle
$$

$$
\begin{aligned}
|\phi_1\rangle &= \frac{1}{\sqrt{3}}(|4\rangle + |5\rangle + |6\rangle) \\
|\phi_2\rangle &= \frac{1}{\sqrt{3}}(|9\rangle + |10\rangle + |11\rangle) \\
|\phi_3\rangle &= \frac{1}{\sqrt{3}}(|1\rangle + |2\rangle + |3\rangle) \\
|\phi_4\rangle &= \frac{1}{\sqrt{2}}(|7\rangle + |8\rangle)
\end{aligned}
\tag{51}
$$

So

$$
\begin{aligned}
A_{H_2}|\phi_0\rangle &= \sqrt{3}|\phi_1\rangle \\
A_{H_2}|\phi_1\rangle &= \sqrt{3}|\phi_0\rangle + 2|\phi_1\rangle + 2|\phi_2\rangle + 3|\phi_3\rangle \\
A_{H_2}|\phi_2\rangle &= 2|\phi_1\rangle + |\phi_3\rangle \\
A_{H_2}|\phi_3\rangle &= 3|\phi_1\rangle + |\phi_2\rangle + 2|\phi_3\rangle + \sqrt{6}|\phi_4\rangle \\
A_{H_2}|\phi_4\rangle &= \sqrt{6}|\phi_3\rangle
\end{aligned}
\tag{52}
$$

$$
A_{H_2} = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 & 0 \\ \sqrt{3} & 2 & 2 & 3 & 0 \\ 0 & 2 & 0 & 1 & 0 \\ 0 & 3 & 1 & 2 & \sqrt{6} \\ 0 & 0 & 0 & \sqrt{6} & 0 \end{pmatrix}
\tag{53}
$$

By some calculations, we see that

$$
\langle\phi_0|e^{-iA_{H_1}t} - e^{-iA_{H_2}t}|\phi_0\rangle =
$$

$$
0.0655e^{2.7913it} - 0.1067e^{1.4051it} - 0.0655e^{-1.7913it} + 0.1067e^{-6.4051it}
$$

$$
\langle\phi_1|e^{-iA_{H_1}t} - e^{-iA_{H_2}t}|\phi_0\rangle =
$$

$$
-0.1091e^{2.7913it} + 0.32e^{1.4051it} + 0.1091e^{-1.7913it} - 0.32e^{-6.4051it}
$$

$$
\langle\phi_2|e^{-iA_{H_1}t} - e^{-iA_{H_2}t}|\phi_0\rangle =
$$

$$
0.0259e^{2.7913it} - 0.32e^{1.4051it} - 0.0218e^{-1.7913it} + 0.32e^{-6.4051it}
$$

$$
\langle\phi_3|e^{-iA_{H_1}t} - e^{-iA_{H_2}t}|\phi_0\rangle =
$$

$$
-0.1091e^{2.7913it} + 0.32e^{1.4051it} + 0.1091e^{-1.7913it} - 0.32e^{-6.4051it}
$$

$$
\langle\phi_4|e^{-iA_{H_1}t} - e^{-iA_{H_2}t}|\phi_0\rangle =
$$

$$
0.1309e^{2.7913it} - 0.2133e^{1.4051it} - 0.1309e^{-1.7913it} + 0.2133e^{-6.4051it}
$$

The amplitudes of single particle quantum walk are different for two nonisomorph graphs. Therefore the single particle quantum walk can distinguish graph nonisomorphism.

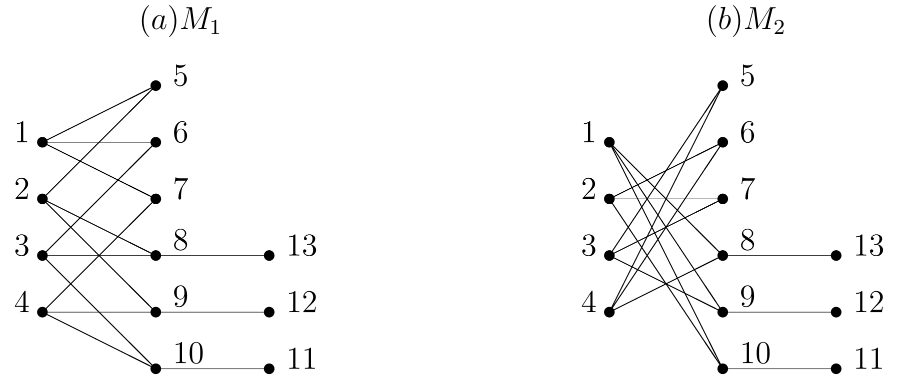

Figure 4 A pair of nonisomorphic cospectral graphs.(a) : M_1 and (b) : M_2. Single particle quantum walk can distinguish these two graphs.

Example III: Two graphs M_1 and M_2 in the Fig (4) are cospectral and nonisomorph. They have 13 vertices and 15 edges. The degree distribution of two graphs are

$$3, 3, 3, 3, 2, 2, 2, 3, 3, 3, 1, 1, 1$$

The stratification basis are defined in the graph M_1 as following

$$|\phi_0\rangle = |1\rangle$$

$$|\phi_1\rangle = \frac{1}{\sqrt{3}}(|5\rangle + |6\rangle + |7\rangle)$$

$$|\phi_2\rangle = \frac{1}{\sqrt{3}}(|2\rangle + |3\rangle + |4\rangle)$$

$$|\phi_3\rangle = \frac{1}{\sqrt{3}}(|8\rangle + |9\rangle + |10\rangle)$$

$$|\phi_4\rangle = \frac{1}{\sqrt{3}}(|11\rangle + |12\rangle + |13\rangle) \tag{54}$$

So

$$A_{M_1}|\phi_0\rangle = \sqrt{3}|\phi_1\rangle$$

$$A_{M_1}|\phi_1\rangle = \sqrt{3}|\phi_0\rangle + |\phi_2\rangle$$

$$A_{M_1}|\phi_2\rangle = |\phi_1\rangle + 2|\phi_3\rangle$$

$$A_{M_1}|\phi_3\rangle = |\phi_4\rangle + 2|\phi_2\rangle$$

$$A_{M_1}|\phi_4\rangle = |\phi_3\rangle \tag{55}$$

$$A_{M_1} = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 & 0 \\ \sqrt{3} & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 2 & 0 \\ 0 & 0 & 2 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad (56)$$

The stratification basis are defined in the graph M_2 as following

$$\begin{aligned} |\phi_0\rangle &= |1\rangle \\ |\phi_1\rangle &= \frac{1}{\sqrt{3}}(|8\rangle + |9\rangle + |10\rangle) \\ |\phi_2\rangle &= \frac{1}{\sqrt{3}}(|2\rangle + |3\rangle + |4\rangle) \\ |\phi_3\rangle &= \frac{1}{\sqrt{3}}(|5\rangle + |6\rangle + |7\rangle) \\ |\phi_4\rangle &= \frac{1}{\sqrt{3}}(|11\rangle + |12\rangle + |13\rangle) \end{aligned} \quad (57)$$

So

$$\begin{aligned} A_{M_2}|\phi_0\rangle &= \sqrt{3}|\phi_1\rangle \\ A_{M_2}|\phi_1\rangle &= \sqrt{3}|\phi_0\rangle + |\phi_2\rangle + |\phi_4\rangle \\ A_{M_2}|\phi_2\rangle &= |\phi_1\rangle + 2|\phi_3\rangle \\ A_{M_2}|\phi_3\rangle &= 2|\phi_2\rangle \\ A_{M_2}|\phi_4\rangle &= |\phi_1\rangle \end{aligned} \quad (58)$$

$$A_{M_2} = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 & 0 \\ \sqrt{3} & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 2 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix} \quad (59)$$

The difference between amplitudes of single particle quantum walk for two graphs are

$$\langle\phi_0|e^{-iA_{M_1}t} - e^{-iA_{M_2}t}|\phi_0\rangle =$$

$$0.6554e^{2.5616it} + 0.1492e^{1.5616it} - 0.1875 + 0.1492e^{-1.5616it} - 0.0555e^{-2.5616it}$$

$$\langle\phi_1|e^{-iA_{M_1}t} - e^{-iA_{M_2}t}|\phi_0\rangle =$$

$$-0.1212e^{2.5616it} + 0.1212e^{1.5616it} + 0.1212e^{-1.5616it} - 0.1212e^{-2.5616it}$$

$$\langle\phi_2|e^{-iA_{M_1}t} - e^{-iA_{M_2}t}|\phi_0\rangle =$$

$$0.0554e^{2.5616it} - 0.1492e^{1.5616it} + 0.1875 - 0.1492e^{-1.5616it} - 0.1875e^{-2.5616it}$$

$$\langle\phi_3|e^{-iA_{M_1}t} - e^{-iA_{M_2}t}|\phi_0\rangle =$$

$$0.1212e^{2.5616it} - 0.1212e^{1.5616it} - 0.1212e^{-1.5616it} + 0.1212e^{-2.5616it}$$

$$\langle\phi_4|e^{-iA_{M_1}t} - e^{-iA_{M_2}t}|\phi_0\rangle = 0$$

The amplitudes of single particle quantum walk are different for two nonisomorph graphs. Therefore the single particle quantum walk can distinguish graph nonisomorphism.

5 Conclusion

We investigated the graph isomorphism problem, in which one wishes to determine whether two graphs are isomorphic. In two non-isomorph cospectral graphs $G_4(n, n+2)$ and $G_5(n, n+2)$, we used n-particle quantum walk to distinguish these two graphs. It was performed by using the antisymmetric fermionic basis. The adjacency matrices of graphs was written in these new basis. The amplitudes of n-particle quantum walk, were different for two graphs, so the multiparticle quantum walk could detect non-isomorph pairs. In the process of fermionization of basis, the complexity has been reduced. Also in two other similar cases $T_4(n, n+2)$ and $T_5(n, n+2)$, the n-particle quantum walk could detect these graphs. It was shown that n-particle quantum walk can detect non-isomorph pairs of $G_4(n, n+2)$ and $G_5(n, n+2)$. In some examples of non-isomorph cospectral graphs, we show that the single particle quantum walk can detect non-isomorphism.

One expect that the quantum walk in antisymmetric basis be able to distinguish some other kinds of graphs. Also it seems that the entanglement entropy is a powerful tool for detecting non-isomorph graphs.

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