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On the tailed model of quantum walks

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Abstract

In this thesis, we examine the tailed model of quantum walks. Unlike the usual quantum walks, the tailed model guarantees the convergence of the state of the walker to a stationary state. The purpose of this study is to study how we can utilize this converging property of our model in various ways. We consider two types of quantum dynamics, the Szegedy dynamics and a Grover-like dynamics. We obtain the scattering of the walk for these two dynamics in the long run, and based on the scattering matrix in the latter case, we obtain a characterization of bipartite graphs. Moreover, we show that, in the Szegedy walk case, the stationary state expresses an electric current function which satisfies the Kirchhoff current and voltage laws, and in the Grover-like dynamics, if the underlying graph is (non-)bipartite, the stationary state expresses a (pseudo-)current function which satisfies (pseudo-)Kirchhoff laws. Furthermore, in the Grover-like case, we introduce a quantum analogy of the electrical energy, called 'comfortability' and we show that the comfortability of the underlying graph can be expressed in terms of the combinatorial properties of the graph. Finally, we discuss a quantum search algorithm on complete graphs, which gives two types of finding probabilities, a maximum probability which is similar to the usual quantum search algorithms and a converging finding probability which arises from the converging property in our model.

Contents

Chapter 1

Introduction

1.1 Discrete time quantum walks

Discrete time quantum walks are studied in different aspects, many interesting behaviours and results of them are derived. Compared to the random walks, quantum walks achieve a quantum speedup in algorithms, such as the quantum walk based search algorithm. Other than the search algorithms, quantum walks are useful in many aspects in computing, such as graph characterizations, graph isomorphism problem, triangle problem and element distinction problem[18, 21, 25].

As discrete-time quantum walks on graphs are being studied, many interesting behaviors of quantum walks, which cannot be observed in the classical random walk setting, have become apparent: the accomplishment of quantum speed up in quantum algorithm, linear spreading, localization, periodicity, pseudo-perfect state transfer and so on (see [16, 18, 21] and references therein). Among them it is revealed that behaviors of quantum walks are closely related to geometric features of graphs; for example, cycle geometry of graphs gives the localization [11, 13], a three-edge-coloring induces an eigenfunction of some quantum walks [19], and the rotation systems and 1-factorizations of graphs are reflected on the mixing time of quantum walks [9]. In this paper, we observe what property of graphs are extracted from the structure of the stationary state of quantum walks. The stationary state, which is a kind of the long time behavior of quantum walk, has been discussed in [7, 8, 14]. The stationary state of the walk produces some interesting results, which don't appear in the usual quantum walks, such as the global scattering of the walk and the induced current function [14]. In this thesis, we emphasise the fact that, the state of the quantum walk model we introduce in the next paragraph converges to a stationary state and for the rest of the thesis, we work on several problems on *how to utilize the stationary state of the walker in various aspects?*

Let us explain our setting and motivation to focus on stationary states. For a connected and locally finite graph $G = (V, E)$, which may be infinite, let us define the set of symmetric arcs A induced by E as follows: for any undirected edge $e \in E$ with end vertices $u, v \in V$, the induced arcs are a and $\overline{a}$, which are arcs from u to v and v to u along the edge $e \in E$, respectively. The terminus and origin vertices of $a \in A$ are denoted by $t(a)$, $o(a) \in V$, respectively. The total space of quantum walk treated here is denoted by $\mathbb{C}^A$, which is the vector space of complex-valued functions on A. Let $\delta_a(\cdot)$ be the delta function such that

$$\delta_a(a') = \begin{cases} 1 & \text{if } a = a', \\ 0 & \text{otherwise.} \end{cases}$$

The time evolution operator of a quantum walk $U : \mathbb{C}^A \to \mathbb{C}^A$ is defined by

$$U = SC.$$

Here $S\delta_a = \delta_{\overline{a}}$ and $C = \bigoplus_{v \in V} C_v$, where C_v is a local coin operator assigned at vertex v which is a $\deg(v)$-dimensional unitary matrix on $\operatorname{span}\{\delta_a : t(a) = v\}$. Note that the time evolution operator U is unitary in the sense that $UU^* = I$. Let ψ_n be the n-th iteration of U with the initial state ψ_0; that is, $\psi_{n+1} = U\psi_n$. We call for any $a \in A$, $\psi_\infty(a) := \lim_{n\to\infty} \psi_n(a)$, if it exists, the stationary state. Another type of stationarity of quantum walks, the stationary *measure*, is discussed in [17], whose form is as follows: $\Phi(\psi_{n+1})(u) = \sum_{t(a)=u} |\psi_{n+1}(a)|^2 = \sum_{t(a)=u} |\psi_n(a)|^2$ for any time step $n = 0, 1, 2, \ldots$ and vertex $u \in V$.

We are interested in how the state converges to the stationary state as a fixed point of a dynamical system. In general, the state of the walker in a quantum walk on a finite graph does not necessarily converge because the time evolution operator is unitary and hence the absolute values of the eigenvalues of the operator are equal to 1. When semi-infinite length paths are connected to a finite graph and the l^∞-initial state is set so that quantum walkers along the tails come into the internal and quantum walkers go out from that at every time step, the convergence of states are shown in [7, 8, 14]. In this setup, the state space of the walk is described by l^∞-space. This quantum walk always converges to a stationary state independent of the choice of the vertices of the internal graph, to which the semi-infinite length paths are connected. In [14], the Grover walk is studied, in which the local coin operators are described by the *Grover operator.*

Definition 1.1 (Grover operator)**.** *The Grover operator $Gr(r)$ is an $r \times r$ matrix defined by*

$$(Gr(r))_{a,b} = \frac{2}{r} - \delta_{a,b}.$$

Let $\tilde{A}$ be the set of arcs in the graph obtained by connecting tails and ψ_t be the state of the walker at time step t. Then the following theorem holds.

Theorem 1.2 (See [14])**.** *In the above setting, if unitary operator U is described by the Grover operator at each vertex, that is $C_v = Gr(deg(v))$, and the initial state is chosen so that the probability amplitudes on the arcs of the j-th tail which are coming towards the internal graph are α_j and 0 elsewhere, then*

$$\psi_\infty := \lim_{t\to\infty} \psi_t$$

exists. Here the limit denotes the point-wise convergence.

This theorem obtained in [14] is remarkably useful and opens a path to obtain many interesting results. For example, noting that, the stationary state is a fixed point to the unitary operator, we can obtain the scattering matrix of the walk.

Definition 1.3 (Scattering Matrix)**.** *Let $A_{in} = \{a_1, \cdots, a_r\}$ be the set of arcs on the tails where $t(a_j)$ are in the internal graph and $A_{out} = \{a : \overline{a} \in A_{in}\}$. Let $\boldsymbol{\alpha} = [\alpha_1, \cdots, \alpha_r]^\top$ and $\boldsymbol{\beta} = [\beta_1, \cdots, \beta_r]^\top$ where $\alpha_j = \psi_\infty(a_j)$ and $\beta_j = \psi_\infty(\overline{a_j})$. Then the scattering matrix σ is an $r \times r$ matrix which satisfies*

$$\boldsymbol{\beta} = \sigma\boldsymbol{\alpha}$$

for any choice of $\boldsymbol{\alpha}$.

In the case of Grover walks, the following theorem for the scattering matrix is known.

Theorem 1.4. *Let $A_{in}, A_{out}, \boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ be defined as in definition 1.3 and the unitary operator is described by the Grover operator. Then the scattering matrix σ which satisfies the equation $\boldsymbol{\beta} = \sigma\boldsymbol{\alpha}$ is given by*

$$\sigma = Gr(r)$$

It can be noted that the scattering matrix in the above case does not contain any information about the internal graph. In a similar way, we study the quantum walk for the case when the time evolution operator is described by the *Szegedy matrix* and we obtain the scattering matrix in chapter 2.

Definition 1.5 (Szegedy matrix)**.** *For a unit vector $\boldsymbol{v} \in \mathbb{C}^r$ the Szegedy matrix with respect to $\boldsymbol{v}$ is defined by*

$$Sz(\boldsymbol{v}) = 2\boldsymbol{v}\boldsymbol{v}^* - I.$$

Here, I is the identity matrix.

In the next chapter, we define the Szegedy matrix in terms of a given probability function p, and we show that the stationary state ψ_∞ exists. As in [14], we can get use of this stationary state to find the scattering matrix in the long run.

As mentioned earlier, in [12, 14], the Grover walk whose quantum coins are expressed by the Grover matrices $\{\mathrm{Gr}(\deg(u))\}_{u\in V}$ was applied with the constant inflow. Then the scattering on the surface in the long time limit recovers the local scattering at each vertex; that is, the scattering matrix is $\mathrm{Gr}(r)$, where r is the number of tails. This implies that we can obtain the global scattering by only some information on the surface, the number of tails connected to the internal graph G_0, whereas this also implies that we cannot obtain any information on the structure of the internal graph G_0. To investigate how the geometrical structure of the internal graph affects the behavior of quantum walkers in terms of their stationary states, we must change something in our setting; for example, we replace a constant flow with some oscillated one. In chapter 3, we show that this change in the input is equivalent to a change in the dynamics, which is called a *Grover-like dynamics* in this thesis, and the quantum walk model with this new dynamics is called *the defective model.* We note that the defective model is a special case of the model studied in [14], and hence some information on our new quantum walk model is readily available, for example, the existence of the stationary state ψ_∞. As our interest revolves around the uses of the stationary state, we compute the scattering matrix of our walk in the long run, and surprisingly, our expected goal of obtaining information about the structure of the internal graph is achieved. Let us present the corresponding theorem as follows, leaving the detailed proof of the theorem to Chapter 3.

Theorem 1.6. *Let $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ represent the inflow and outflow of the stationary state on the surface. Then we have*

$$\boldsymbol{\beta} = \sigma\boldsymbol{\alpha},$$

where the scattering matrix σ is unitary and described by

$$\sigma = \begin{cases} I & : G_0 \text{ is non-bipartite,} \\ \tau & : G_0 \text{ is bipartite.} \end{cases}$$

Here τ is described as follows:

$$\tau = -\begin{bmatrix} I_k & 0 \\ 0 & -I_{r-k} \end{bmatrix} \mathrm{Gr}(r) \begin{bmatrix} I_k & 0 \\ 0 & -I_{r-k} \end{bmatrix},$$

where k and $r-k$ are the numbers of tails connected to each partite set in the internal graph G_0.

From this theorem, if the interior is non-bipartite, the scattering is the perfect reflection, while if the interior is bipartite, the scattering is described by the Grover matrix. We remark that this theorem gives a characterization of bipartite graphs, and the rest of the chapter 3 flows based on this characterization.

Another remark we make on this theorem is that it can be used to characterize the disconnected graphs in some special situations. For example, if the scattering matrix is in the form of a block diagonal matrix

$$\sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ 0 & \cdots & 0 & \sigma_s \end{bmatrix},$$

where at least one of σ_j is of the form τ then the underlying graph is disconnected. In particular, if all of them are of the form τ then the underlying graph is disconnected with s number of components. On the other hand, If $\sigma = I$ then the above theorem does not provide any information about the connectedness of the graph.

Now let us explain some background on the scattering we study here. In [20], a discrete-time quantum walk model on $\mathbb{Z}$ is studied and it is observed that this model behaves like a quantum tunnel with a tunneling effect: i.e. the quantum mechanical phenomenon where the particles succeed in passing through a potential barrier. This paper discussed the conditions when a perfect transmission occurs through a *double-well*. This double-well is replaced by a finite graph in [14] and the model now becomes a quantum walk on a finite graph with two infinite tails where in the stationary state, the perfect transmission occurs. Furthermore, the model is generalized by adding an arbitrary number of tails and hence, the perfect transmission changes into a scattering in the stationary state.

Another interesting result obtained in [14] is a type of a current function obtained in terms of the stationary state. In literature, for example in [3, 4, 2, 22], the algebraic models of electric networks are well studied. These electrical networks can be formulated using the incidence and Laplacian matrices of the underlying graphs.

1.2 Electrical networks

Let G be the underlying graph of an electric circuit with vertex set $V = \{v_1, ..., v_n\}$ and edge set $E = \{e_1, ..., e_m\}$ where the edges are labelled so that $e_1, ..., e_{n-1}$ are the edges of a given spanning tree T of G. For each edge $e = \{u, v\}$, choose one of the vertices u, v to be the positive end of e and the other vertex to be the negative end. Then we say that the graph is given an orientation. For a given orientation, the incidence matrix $D = (d_{i,j})$ is defined by

$$d_{i,j} = \begin{cases} 1 & \text{if } v_i \text{ is the positive end of } e_j, \\ -1 & \text{if } v_i \text{ is the negative end of } e_j, \\ 0 & \text{otherwise.} \end{cases}$$

The incidence matrix D of G defined above can be partitioned as follows.

$$D = \begin{bmatrix} D_T & & D_N \\ & d_n & \end{bmatrix}$$

where D_T is an $(n-1) \times (n-1)$ matrix and d_n is a row matrix which is linearly dependent on the other rows. By [3, Proposition 5.4] it follows that D_T is invertible. Let $C_T = -D_T^{-1} D_N$. Define the matrix C by

$$C = \begin{bmatrix} C_T \\ I_{m-n+1} \end{bmatrix}$$

Now consider the case when each edge e_i in the graph has conductance M_i. Let $M := \mathrm{diag}(M_1, \cdots, M_m)$, a diagonal matrix whose diagonal elements are the corresponding conductances, then the current vector w, voltage vector z and the vector of externally applied voltages α defined on E which are related by the equation $z = Mw + \alpha$ satisfy the following laws of electric circuits which are called the *Kirchhoff's laws.*

1. *Kirchhoff's Current Law (KCL):*
$$Dw = 0$$

2. *Kirchhoff's Voltage Law (KVL):*
$$C^\top z = 0$$

In other words, KCL is the rule which says that for every vertex u in the underlying graph G, the total current entering u is equal to the total current leaving u, and KVL is the rule which says that for any cycle in the underlying graph G, the total current along the cycle is 0. Here, C is constructed so that the columns of C corresponds to the vectors in the cycle subspace of the graph [3].

For simplicity, let us assume that each edge has conductance 1. By [3, Additional results 4a], there exists a potential function ϕ defined on V such that $z = D^\top \phi$. Then the equation $z = w + \alpha$ becomes $D^\top \phi = w + \alpha$ which implies

$$L\phi = \eta,$$

where $L := DD^\top$ is the Laplacian matrix of G and $\eta := D\alpha$ is the vector whose entry labeled by v, η_v is the current flowing into the network at the vertex v. This is called the *Laplacian formulation of network equations*[3].

Now let us turn back to the quantum walk model with tails. As mentioned earlier, the stationary state ψ_∞ exists, and define a function $j(\cdot)$ as follows.

$$j(a) := \psi_\infty(a) - \frac{1}{r}\sum_{k=1}^{r} \alpha_k$$

Then the following theorem holds.

Theorem 1.7 (See [14])**.** *If $j(\cdot)$ is defined as above, then $j(\cdot)$ expresses a current flow.*

In other words, the function $j(\cdot)$ satisfies the following Kirchhoff's laws

1. *Kirchhoff's Current Law:*

$$\sum_{b\in\tilde{A}:t(b)=u} j(b) = 0;\ j(a) + j(\overline{a}) = 0,\ (u \in \tilde{V}, a \in \tilde{A}).$$

2. *Kirchhoff's Voltage Law:*
For any cycle $c = (a_1, ..., a_s)$ with $t(a_1) = o(a_2), ..., t(a_{s-1}) = o(a_s), t(a_s) = o(a_1)$ in G_0, it holds

$$\sum_{k=1}^{s} j(a_k) = 0.$$

In this thesis, we first study in chapter 2, a current function which arises from the stationary state in the case of the Szegedy walk. We obtain a current function $j(\cdot)$ in terms of the stationary state and show that it satisfies the Kirchhoff's current and voltage laws. In chapter 3, we study the Grover walk and we focus on the simplest oscillation of inflow with alternating signs which is a coarse graining of alternating current input. This setup gives a characterization of bipartite graphs and based on this characterizattion, we define a current and a pseudo-current function which satisfy the Kirchhoff and a kind of a psudo-Kirchhoff laws respectively. Moreover, we express these results in terms of the Laplacian and signless-Laplacian matrices of the underlying graphs respectively.

As mentioned earlier, the scattering matrix gives an information about the surface or the boundary of the graph. Next it is natural to ask what happens to the interior. To answer this question, we introduce the idea of comfortability. The comfortability is a function of the interior, and gives how quantum walkers accumulate in the internal graph in the long time limit, which is the energy stored the interior. The detailed definition of the comfortability $\mathcal{E}_{QW}(G_0)$ is described in Definition 3.3. We obtain that when only two tails are connected, the comfortability of the graph can be expressed in terms of the geometric information of the graph as follows.

Theorem 1.8. *Assume the number of tails is 2, and the inflow $\boldsymbol{\alpha} = (\alpha_1, \alpha_2)^\top = (1, 0)^\top$. Then the comfortability $\mathcal{E}_{QW}(G_0)$ of the quantum walk is given by*

$$\mathcal{E}_{QW}(G_0) = \begin{cases} \dfrac{1}{4}\left(\dfrac{\chi_2(G_0)}{\chi_1(G_0)} + |E_0|\right) & : G_0 \text{ is bipartite,} \\ \\ \dfrac{\iota_2(G_0)}{\iota_1(G_0)} & : G_0 \text{ is non-bipartite.} \end{cases}$$

Here $|E_0|$ is the number of edges of G_0, $\chi_1(G_0)$ is the tree number of G_0, that is the number of the spanning trees of G_0 and $\chi_2(G_0)$ is the number of the spanning forests of G_0 with two components in which one contains u_1 and the other contains u_n. Here u_1 and u_n are the vertices in G_0 where the tails with the inflows α_1 and α_2 are connected respectively. The geometric quantities of $\iota_1(G_0)$ and $\iota_2(G_0)$ are defined in Section 3.

We illustrate the ranking of the comfortability among all of the graphs with four vertices in Section 3.6. To show the above theorem, we first define a (pseudo-)current function [12, 14] on a (non-)bipartite graph and we show that these functions satisfy the (pseudo-)Kirchhoff laws in Theorems 3.6 and 3.7, respectively. Secondly, we obtain a potential function with respect to these (pseudo-)current functions, in terms of (signless-)Laplacian matrix in [3, 4] and Theorem 3.9, respectively. Thirdly, using these expressions of the potential functions, we obtain expressions for the comfortability in terms of the (non-)oriented incident matrix and the (signless-)Laplacian matrix, when the graph is (non-)bipartite in Propositions 3.12 and 3.13. Finally, using the speciality of the setting, we obtain the expression of the comfortability using the graph factors induced quantum walks defined by Definition 3.10.

A similar notion of extracting the combinatorial information of the underlying graph in an electric network can be found in literature, for example in [2]. For an electric network on the underlying graph G_0 with the given inductance, resistance and capacitance on each edge, the Laplace transformed network equations are used to find the resultant impedance between the input and the output vertices u_1 and u_n in terms of the combinatorial properties of G_0. For example, the impedance of an electric network between the vertices u_1 and u_n can be found using the following theorem. Here we assume that the resistance on each edge is 1 for simplicity.

Theorem 1.9. *(See [2, Section 3.8]) The impedance Z of the electric circuit is given by*

$$Z = \frac{\chi_2(G_0)}{\chi_1(G_0)}$$

where $\chi_1(G_0)$ is the tree number of G_0, that is the number of the spanning trees of G_0 and $\chi_2(G_0)$ is the number of the spanning forests of G_0 with two components in which one contains u_1 and the other contains u_n.

1.3 Quantum search algorithms

Quantum walk based search algorithm is a popular area of study in quantum walks. For a given graph G, the problem is to search a specific set of vertices of G. For simplicity, let the size of this set be 1, that is the problem is to search a given vertex u_* of G, where the number of vertices of G is N. In the classical case, the run-time of the search algorithms are of the order $O(N)$. With the quantum walk based search algorithms, the vertex u_* can be searched in the run-time of the order $O(\sqrt{N})$, that is, the quantum walk based search algorithm gives a quadratic speed up.

Let us explain the search algorithm based on the *Grover operator*, which is related to chapter 4 in this thesis. Let G be a graph with the set of vertices V, the set of edges E and the set of arcs induced by E is A. Let M be the set of marked vertices, which are to be searched. Define the coin operator $C = \bigoplus_{v \in V} C_v$ as follows.

$$C_v = \begin{cases} -G_v & \text{if } v \in M \\ \\ G_v & \text{if } v \in V \setminus M \end{cases}$$

where G_v is the Grover operator on the vertex v. In particular, let $M = \{u_*\}$, then the time evolution operator U' can be written as

$$U' = UR$$

where U is the time evolution operator described by the Grover operator defined at each vertex of G and R is the operator given as follows.

$$R = I - 2 \sum_{a:t(a)=u_*} |a\rangle \langle a| \,.$$

By choosing the initial state as

$$\Psi_0 = \frac{1}{\sqrt{|A|}} \sum_{a \in A} |a\rangle \,,$$

the time evolution operator U' is applied t times to obtain the state Ψ_t of the walker at the time step t. The finding probability of u_* at time step t is given by

$$p_t(u_*) = \sum_{a:t(a)=u_*} |\Psi_t(a)|^2.$$

The problem is to find the optimal time t_{opt} such that the finding probability $p_{t_{opt}}(u_*)$ is maximum, which is called the success probability denoted by p_{succ}.

It is known (by [21]) that applying the search algorithm to the complete graph with N number of vertices, choosing the optimal time t_{opt} to be

$$t = \lfloor \frac{\pi}{4}\sqrt{N} \rfloor$$

and measuring the state of the walker, the marked vertex u_* can be searched with a success probability p_{succ} given by

$$p_{succ} = 1 + O(\frac{1}{N}).$$

Moreover in [23], it is proved that if the above time evolution operator U' is applied to the above initial state Ψ_0 on a hypercube with $N = 2^n$ number of vertices, the optimal run-time of the algorithm to search the marked vertex u_* is given by

$$t_{opt} = \lfloor \frac{\pi}{2}\sqrt{N} \rfloor$$

and the success probability is given by

$$p_{succ} = \frac{1}{2} + O(\frac{1}{n}).$$

Furthermore, it is known by [24] that the quantum search algorithm on a Johnson graph $J(n,k)$ has a success probability

$$p_{succ} = \frac{1}{2} + O(\frac{1}{\sqrt{n}})$$

at the optimal run-time

$$t_{opt} \approx \frac{\pi}{2\sqrt{2}}\sqrt{N}.$$

These results show that the quantum search algorithm on above graphs has a quadratic speed-up and the optimal run-time is of the order $O(\sqrt{N})$. Similar to these results, we study in chapter 4, the quantum search of a given vertex in a complete graph with N vertices, where infinite tails are connected to the graph. As our intuition suggests, we show that the optimal run-time of the algorithm is of the order $t_{opt} = O(\sqrt{N})$ and the success probability satisfying $p_{succ} > \frac{1}{2}$.

In addition to that, since the state of the walker converges in our model, it is natural to arise the question *"What would it be the finding probability in the long run?"* To answer this question, we study the limit of the finding probability in the long run. In chapter 4, we show that

$$\lim_{t\to\infty} p_t(u_*) = \frac{1}{2}.$$

Moreover, by obtaining $\|\Psi_\infty - \Psi_t\|$, we show that the finding probability p_t becomes arbitrary close to $\frac{1}{2}$ while the run-time of the algorithm is set to the order $O(N \log N)$. This result implies that the tailed model we define gives two types of finding probabilities, a maximum finding probability at the run-time of the order $O(\sqrt{N})$ and a finding probability in the stationary state, which is at a run-time $O(N \log N)$.

With the use of these notion, we arrange the rest of the thesis as follows. In chapter 2, we study the Szegedy walk on the tailed model. We obtain the scattering matrix in the long run, and in the stationary state, we derive an electric current function which satisfies the Kirchhoff's current and voltage laws.

In chapter 3, we study a Grover-like dynamics on the tailed model. First we show that in our setting, we can obtain a characterization of bipartite graphs by finding the scattering matrix and the rest of the chapter is based on this characterization. In the stationary state, we derive a current function and a pseudo-current function in the case when the underlying graph is bipartite and non-bipartite respectively, which satisfies the Kirchhoff's laws and pseudo-Kirchhoff laws respectively. Moreover, we formulate these network equations using the Laplacian and signless-Laplacian matrices of the underlying graph respectively. Furthermore, we introduce the notion of comfortability, an analogy of the electrical energy and using the properties of Laplacian and signless-Laplacian matrices, we obtain the comfortability of the underlying graph in terms of the combinatorial properties of the graph. In particular, if the underlying graph is bipartite, we show that the comfortability of the underlying graph can be obtained in terms of the tree number and the number of spanning forests, and if the underlying graph is non-bipartite, we show that the comfortability can be obtained in terms of spanning unicyclic subgraphs.

Finally, in chapter 4, we study a quantum search algorithm on complete graphs. Here we show that there are two types of finding probabilities, a maximum finding probability as in the usual quantum walks at the run-time of the order $O(\sqrt{N})$ and a finding probability in the long run, which is at a run-time $O(N \log N)$ which arises from the converging property in our tailed model.

Chapter 2

Electric circuit induced by quantum walks

2.1 Setting

In this section, we study the Szegedy walk in the tailed model. We show that the state of the walker converges in the long run and in this converging state, we derive the scattering matrix of the walker. Moreover, if the underlying random walk is reversible, then we define an electric current function, which satisfies the Kirchhoff's current and voltage laws.

Now let us explain the setting of the quantum walk. Let $G_0 = (V_0, E_0)$ be a finite connected graph and A_0 be the symmetric arc set induced by E_0. We choose the boundary of G_0, $\emptyset \neq \delta V \subset V_0$ with $\delta V = \{v_1^{(0)}, ..., v_r^{(0)}\}$, where $v_i^{(0)} \neq v_j^{(0)}$ if and only if $i \neq j$. Let $\{\mathbb{P}_j : j = 1, ..., r\}$ be the set of semi-infinite length paths called the tails whose end vertices are $v_j^{(0)}$, connected to the finite graph G_0 such that $V(\mathbb{P}_j) = \left\{v_j^{(0)} \sim v_j^{(1)} \sim v_j^{(2)} \sim ...\right\}$. Here $u \sim v$ means that the vertices u and v are adjacent. We denote the constructed graph by $\tilde{G} = (\tilde{V}, \tilde{E})$. We also denote the arc set induced by E_0 and $\tilde{E}$ by A_0 and $\tilde{A}$ respectively. For any arc $a = (u, v) \in \tilde{A}$, we write $\overline{a} = (v, u)$, $o(a) = u$ and $t(a) = v$. Remark that $o(\overline{a}) = t(a)$ and $t(\overline{a}) = o(a)$.

Set $p : \tilde{A} \to (0, 1]$ such that

$$\sum_{o(a)=u} p(a) = 1, \ (u \in \tilde{V});$$

$$p(a) = 1/2, \ (a \in \cup_{j=1}^{r} A(\mathbb{P}_j) \setminus \overline{\delta A}).$$

Here $\overline{\delta A} := \{a \in \tilde{A} : o(a) \in V_0, t(a) \in \tilde{V} \setminus V_0\}$. The total state space associated with the quantum walk treated here is $\mathbb{C}^{\tilde{A}}$. We define the time evolution operator U on $\mathbb{C}^{\tilde{A}}$ in the matrix form by

$$(U\Psi)(a) = \sum_{b \in \tilde{A}: t(b) = o(a)} (2\sqrt{p(a)p(\overline{b})} - \delta_{\overline{a},b})\Psi(b),$$

for any $\Psi \in \mathbb{C}^{\tilde{A}}$. Note that the walk becomes "free" on the tails; that is,

$$(U)_{a,b} = \begin{cases} 1 & : o(a) = t(b), \ a \neq \overline{b}, \\ 0 & : \text{otherwise} \end{cases}$$

for any $o(a) \notin V_0$. Set the initial state of the walk as

$$\Phi_0(a) = \begin{cases} \alpha_j & \text{if } o(a) = v_j^{(s+1)}, \ t(a) = v_j^{(s)}, \ s = 0, 1, 2, ..., \ j = 1, 2, ..., r, \\ \\ 0 & \text{otherwise.} \end{cases}$$

Let $\chi : \mathbb{C}^{\tilde{A}} \to \mathbb{C}^{A_0}$ be the boundary operator of A_0, defined as for any $\Psi \in \mathbb{C}^{\tilde{A}}$, $(\chi\Psi)(a) = \Psi(a)$ $(a \in A_0)$. The adjoint operator, $\chi^* : \mathbb{C}^{A_0} \to \mathbb{C}^{\tilde{A}}$ is described as follows. For any $\psi \in \mathbb{C}^{A_0}$,

$$(\chi^*\psi)(a) = \begin{cases} \psi(a) & \text{if } a \in A_0, \\ \\ 0 & \text{otherwise.} \end{cases}$$

Remark that $\chi\chi^* : \mathbb{C}^{A_0} \to \mathbb{C}^{A_0}$ is the identity operator on $\mathbb{C}^{A_0}$ and $\chi^*\chi : \mathbb{C}^{\tilde{A}} \to \mathbb{C}^{\tilde{A}}$ is the projection operator on $\mathbb{C}^{\tilde{A}}$ with respect to A_0.

Now we restrict the walk on $\tilde{A}$ to A_0. Let E be the time evolution operator restricted to A_0, that is

$$E = \chi U \chi^*.$$

We put

$$\psi_t := \chi\Psi_t$$

is the restriction of the state on A_0. Observe that we have the following.

$$\begin{aligned} \psi_t &= \chi\Psi_t \\ &= \chi U \Psi_{t-1} \\ &= \chi U \chi^* \chi \Psi_{t-1} + \chi U (1 - \chi^*\chi)\Psi_{t-1} \\ &= E\psi_{t-1} + \chi U \Psi_0. \end{aligned}$$

Let $\rho := \chi U \Psi_0$ be the external source to the dynamics of the walk. Then we have

$$\psi_t = E\psi_{t-1} + \rho.$$

By applying an argument to this recursion, similar to the argument in [14], the following theorem holds.

Theorem 2.1. *Let the quantum walk be defined as above. Then there exists* $\Psi_\infty \in \mathbb{C}^{\tilde{A}}$ *such that*

$$\Psi_\infty = \lim_{t\to\infty} \Psi_t.$$

2.2 Scattering matrix

The convergence of the state leads to the scattering matrix of the walker. To find the scattering matrix in the long run, first we give the following lemma.

Lemma 2.2. *For a given probability function* $p : \tilde{A} \to (0, 1]$ *and* $u \in \tilde{V}$, $\dfrac{1}{2\sqrt{p(a)}} (\Psi_\infty(a) + \Psi_\infty(\overline{a}))$ *is constant for all* $a \in \tilde{A}$ *such that* $o(a) = u$.

Proof. It follows from the dynamics of the walk that, in the stationary state, for any $a \in \tilde{A}$,

$$\Psi_\infty(a) = \sum_{b \in \tilde{A}: t(b) = o(a)} 2\sqrt{p(a)p(\overline{b})}\Psi_\infty(b) - \Psi_\infty(\overline{a}).$$

It follows that,

$$\frac{1}{2\sqrt{p(a)}} (\Psi_\infty(a) + \Psi_\infty(\overline{a})) = \sum_{b \in \tilde{A}: t(b) = u} \sqrt{p(\overline{b})}\Psi_\infty(b),\ o(a) = u.$$

Observe that for a given $u \in \tilde{V}$, the right hand side of the equation is a constant. $\square$

Let $\rho_V(u) := \sum_{b\in\tilde{A}:t(b)=u} \sqrt{p(\bar{b})}\Psi_\infty(b)$, then we have

$$\sqrt{p(a)}\rho_V(o(a)) = \frac{1}{2}\left(\Psi_\infty(a) + \Psi_\infty(\overline{a})\right) = \sqrt{p(\overline{a})}\rho_V(t(a))$$

and hence

$$p(a)\rho_V^2(o(a)) = p(\overline{a})\rho_V^2(t(a)).$$

By using the above lemma, we give the proof of the following theorem.

Theorem 2.3. *Assume the underlying random walk is reversible; that is, there exists $m_V \in \mathbb{C}^{\tilde{V}}$ and $m_E \in \mathbb{C}^{\tilde{E}}$ such that*

$$m_E(|a|) = p(a)m_V(o(a)) = p(\overline{a})m_V(t(a)) \neq 0.$$

Here $|a|$ denotes the edge containing the arc a. Let $\boldsymbol{\alpha} := [\alpha_1, \alpha_2, ..., \alpha_r]^T$, $\boldsymbol{\beta} := [\beta_1, \beta_1, ..., \beta_r]^T \in \mathbb{C}^r$, where $\alpha_j = \Psi_\infty(a)$ with $o(a) = v_j^{(1)}$, $t(a) = v_j^{(0)}$ and $\beta_j = \Psi_\infty(a)$ with $o(a) = v_j^{(0)}$, $t(a) = v_j^{(1)}$. Set a unit vector on $\mathbb{C}^r$ by

$$\boldsymbol{m}_{\delta E} := \left[\sqrt{m_E(|a_1|)/m(G_0)}, ..., \sqrt{m_E(|a_r|)/m(G_0)}\right]^T,$$

where $m(G_0) = \sum_{j=1}^{r} m_E(|a_j|)$ and $a_j \in \mathbb{P}_j$ such that $o(a_j) = v_j^{(1)}$, $t(a_j) = v_j^{(0)}$. We define the Szegedy matrix by, for a unit vector $\boldsymbol{v} \in \mathbb{C}^r$, $Sz(\boldsymbol{v}) = 2\boldsymbol{v}\boldsymbol{v}^* - I_{\mathbb{C}^r}$. Then we have

$$\boldsymbol{\beta} = Sz(\boldsymbol{m}_{\delta E})\boldsymbol{\alpha}.$$

Remark. *Here $m_V(u) = \rho_V^2(u)$.*

Proof. Let

$$c_i := \rho_V(u_i) = \sum_{b\in\tilde{A}:t(b)=u_i} \sqrt{p(\bar{b})}\Psi_\infty(b), \tag{2.1}$$

where $u_i = v_i^{(0)}$. Now fix i, and consider the case when the initial state is set to $\alpha_j = \delta_{i,j}$. Let $\Psi_\infty^{(i)}$ and $\beta_{j,i}$ be the stationary state and the transmitting value along $\mathbb{P}_j$ in the stationary state with this initial state respectively. We put $\psi_\infty^{(i)} := \chi\Psi_\infty^{(i)}$. By lemma 2.2, $\beta_{j,i} = 2c_j\sqrt{m_E(|a_j|)} - \delta_{i,j}$. Let

$$A_{in} = \left\{a \in \tilde{A} : o(a) \in \tilde{V} \setminus V_0, t(a) \in V_0\right\},$$
$$A_{out} = \left\{a \in \tilde{A} : \overline{a} \in A_{in}\right\}.$$

Then by applying the time evolution operator once, we get

$$U\left(\Psi_\infty|_{A_{in}} + \Psi_\infty|_{A_0}\right) = \Psi_\infty|_{A_{out}} + \Psi_\infty|_{A_0}.$$

This can be rewritten as

$$U(\chi^*\psi_\infty^{(i)} + |a_i\rangle) = \chi^*\psi_\infty^{(i)} + \boldsymbol{\beta}^{(i)},$$

where $\boldsymbol{\beta}^{(i)} = \sum_{j=1}^{r} \beta_{j,i} |\overline{a_j}\rangle$. Now we have the following.

$$\begin{aligned}\langle\psi_\infty^{(i')}, \psi_\infty^{(i)}\rangle + \langle\boldsymbol{\beta}^{(i')}, \boldsymbol{\beta}^{(i)}\rangle &= \langle\chi^*\psi_\infty^{(i')} + \boldsymbol{\beta}^{(i')}, \chi^*\psi_\infty^{(i)} + \boldsymbol{\beta}^{(i)}\rangle \\ &= \langle\chi^*\psi_\infty^{(i')} + |a_{i'}\rangle, \chi^*\psi_\infty^{(i)} + |a_i\rangle\rangle \\ &= \langle\psi_\infty^{(i')}, \psi_\infty^{(i)}\rangle + \delta_{i',i}\end{aligned}$$

Thus we have

$$\langle\boldsymbol{\beta}^{(i')}, \boldsymbol{\beta}^{(i)}\rangle = \delta_{i',i}$$

which is equivalent to

$$c_i = 0 \text{ or } c_i = \frac{\sqrt{m_E(|a_i|)}}{m(\delta G_0)}.$$

Here $m(\delta G_0) := \sum_{j=1}^{r} m_E(|a_j|)$. Now to obtain the desired result, we show that $c_i \neq 0$. To the contrary let's assume that $c_i = 0$. Then by lemma 2.2 and equation 2.1, $\Psi_\infty^{(i)}(\overline{a}) = -\Psi_\infty^{(i)}(a)$ holds. Moreover, it follows that

$$\sum_{a \in \tilde{A}: t(a)=u} \sqrt{m_E(|a|)}\Psi_\infty^{(i)}(a) = 0$$

for any $u \in \tilde{V}$ and hence

$$\sum_{a \in \tilde{A}: t(a) \in V_0} \sqrt{m_E(|a|)}\Psi_\infty^{(i)}(a) = 0.$$

Therefore it follows that

$$\sum_{a: a \in A_0} \sqrt{m_E(|a|)}\Psi_\infty^{(i)}(a) + 1 = 0.$$

Now by computing $\sum_{a: a \in A_0} \sqrt{m_E(|a|)}\Psi_\infty^{(i)}(a)$ in two ways, we have the following:

$$\begin{aligned}
1 &= -\sum_{a: a \in A_0} \sqrt{m_E(|a|)}\Psi_\infty^{(i)}(a) \\
&= -\sum_{u \in V_0} \sum_{a \in A_0: t(a)=u} \sqrt{m_E(|a|)}\Psi_\infty^{(i)}(a) \\
&= \sum_{u \in V_0} \sum_{a \in A_0: t(a)=u} \sqrt{m_E(|a|)}\Psi_\infty^{(i)}(\overline{a}) \\
&= \sum_{u \in V_0} \sum_{a \in A_0: t(a)=u} \sqrt{m_E(|a|)}\Psi_\infty^{(i)}(a) \\
&= \sum_{a: a \in A_0} \sqrt{m_E(|a|)}\Psi_\infty^{(i)}(a) \\
&= -1
\end{aligned}$$

which is a contradiction and hence

$$c_i = \frac{\sqrt{m_E(|a_i|)}}{m(\delta G_0)}.$$

Thus for any $j = 1, \cdots, r$,

$$\beta_{j,i} = \frac{2}{m(\delta G_0)}\sqrt{m_E(e_i)m_E(e_j)} - \delta_{i,j}.$$

By the linearity of the time evolution, $\boldsymbol{\beta}(j) = \sum_{i=1}^{r} \beta_{j,i}\boldsymbol{\alpha}(i)$ which proves the theorem. □

Now let us consider the case when the underlying random walk is non-reversible. Since $p(a)\rho_V^2(o(a)) = p(\overline{a})\rho_V^2(t(a))$ holds, $\rho_V(u)$ must be 0 for all $u \in \tilde{V}$. This leads to the following theorem.

Theorem 2.4. *Let $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ be the input and output vectors defined in theorem 2.3. If the underlying random walk is non-reversible, then the following holds.*

$$\boldsymbol{\beta} = -\boldsymbol{\alpha}$$

Proof. Since the underlying random walk is non-reversible, $\rho_V(u) = 0$ for all $u \in \tilde{V}$ which implies $\Psi_\infty(a) + \Psi_\infty(\overline{a}) = 0$ for all $a \in \tilde{A}$. In particular, $\Psi_\infty(a_j) = -\Psi_\infty(\overline{a}_j)$ for any $j = 1, \cdots, r$ which implies

$$\boldsymbol{\beta} = -\boldsymbol{\alpha}$$

□

Remark. *We remark that if the random walk is non-reversible, then the following holds.*

$$\sum_{a\in\tilde{A}:t(a)=u} \sqrt{p(\overline{a})}\Psi_\infty(a) = 0,\ (u \in \tilde{V})$$

On the other hand, since the underlying random walk is non-reversible, $p(a) = p(\overline{a})$ is not necessarily true, $\sum_{a\in\tilde{A}:o(a)=u} \sqrt{p(\overline{a})}\Psi_\infty(a) = 0, (u \in \tilde{V})$ is not necessarily true. Hence in the next section, we define a current function, assuming that the underlying random walk is reversible.

2.3 Kirchhoff laws

In this section, we provide an electric current function which satisfies the Kirchhoff's current and voltage laws. In this section, we assume that the underlying random walk is reversible. Before stating the main theorem in this section, we give the following lemma which will be useful in proving the next theorem.

Lemma 2.5. *For any cycle $c = (a_1, ..., a_r)$, the induction function in $\mathbb{C}^{\tilde{A}}$ is denoted by*

$$w_c(a) = \begin{cases} \dfrac{1}{\sqrt{m_E(|a_k|)}} & \text{if } a = a_k, \\ -\dfrac{1}{\sqrt{m_E(|a_k|)}} & \text{if } a = \overline{a}_k, \\ 0 & \text{otherwise,} \end{cases}$$

Then $\langle w_c, \Psi_\infty\rangle = 0$ holds.

Proof. It is easy to check that w_c is an eigenvector of U with the eigenvalue 1, which has the support in A_0. By the proof of the convergence of Ψ_∞, it follows that $\langle w_c, \Psi_\infty\rangle = 0$. □

Now we have the following theorem.

Theorem 2.6. *Let the underlying random walk is reversible. Define $j(\cdot) \in \mathbb{C}^{\tilde{A}}$ by*

$$j(a) := \sqrt{m_E(|a|)}\Psi_\infty(a) - \frac{m_E(|a|)}{\sqrt{m(G_0)}}\langle \boldsymbol{m}_{\delta E}, \boldsymbol{\alpha}\rangle.$$

Then $j(\cdot)$ describes the electric current flow of the following electric circuit: the conductances are assigned at all the edges, and the conductance value at each edge e is given by $m_E(e)$.

Proof. To show that $j(\cdot)$ is an electric current, we show the following Kirchhoff's laws.

1. Kirchhoff's current law:

$$\sum_{t(a)=u} j(a) = \sum_{o(a)=u} j(a) = 0;\ j(a) + j(\overline{a}) = 0;$$

2. Kichhoff's voltage law:

$$\sum_{k=1}^{s} \frac{j(a_k)}{m_E(|a|)} = 0 \text{ for any cycle } c = (a_1, ..., a_s).$$

To show the Kirchhoff's current law, we have

$$\tilde{\rho}_V(u) = \frac{1}{m_V(u)} \sum_{t(a)=u} \sqrt{m_E(|a|)}\Psi_\infty(a) = \frac{1}{\sqrt{m(\delta G_0)}}\langle \boldsymbol{m}_{\delta E}, \alpha_{in}\rangle,$$

which implies

$$\sum_{t(a)=u} \sqrt{m_E(|a|)}\Psi_\infty(a) = \sum_{t(a)=u} \frac{m_E(|a|)}{\sqrt{m(\delta G_0)}} \langle \boldsymbol{m}_{\delta E}, \alpha_{in} \rangle.$$

On the other hand, since $\rho_E(|a|) = \sqrt{m_E(|a|)}\tilde{\rho}_V(o(a))$, we have

$$\rho_E(|a|) = \frac{1}{2}\left(\Psi_\infty(a) + \Psi_\infty(\overline{a})\right) = \frac{\sqrt{m_E(|a|)}}{\sqrt{m(\delta G_0)}} \langle \boldsymbol{m}_{\delta E}, \alpha_{in} \rangle,$$

which implies

$$\sqrt{m_E(|a|)}\left(\Psi_\infty(a) + \Psi_\infty(\overline{a})\right) = \frac{2m_E(|a|)}{\sqrt{m(\delta G_0)}} \langle \boldsymbol{m}_{\delta E}, \alpha_{in} \rangle$$

this implies that

$$\sum_{t(a)=u} j(a) = \sum_{o(a)=u} j(a) = 0; \; j(a) + j(\overline{a}) = 0.$$

To show that $j(\cdot)$ satisfies the Kirchhoff's voltage law, we use lemma 2.5. It holds that

$$\begin{aligned}
\langle w_c, \Psi_\infty \rangle = 0 &\Leftrightarrow \sum_{k=1}^{s} \frac{\Psi_\infty(a_k) - \Psi_\infty(\overline{a}_k)}{\sqrt{m_E(|a_k|)}} = 0 \\
&\Leftrightarrow \sum_{k=1}^{s} \left(\frac{j(a_k)}{m_E(|a_k|)} - \frac{j(\overline{a}_k)}{m_E(|a_k|)} \right) = 0 \\
&\Leftrightarrow \sum_{k=1}^{s} \frac{j(a_k)}{m_E(|a_k|)} = 0
\end{aligned}$$

which concludes the proof. □

Chapter 3

A comfortable graph structure for Grover walk

3.1 Setting

Let $G_0 = (V_0, E_0)$ be a finite connected graph and A_0 be the symmetric arc set induced by E_0. We choose the boundary of G_0, $\emptyset \neq \delta V \subset V_0$ with $\delta V = \{v_1^{(0)}, ..., v_r^{(0)}\}$, where $v_i^{(0)} \neq v_j^{(0)}$ if and only if $i \neq j$. Let $\{\mathbb{P}_j : j = 1, ..., r\}$ be the set of semi-infinite length paths called the tails whose end vertices are $v_j^{(0)}$, connected to the finite graph G_0 such that $V(\mathbb{P}_j) = \left\{v_j^{(0)} \sim v_j^{(1)} \sim v_j^{(2)} \sim ...\right\}$. Here $u \sim v$ means that the vertices u and v are adjacent. We denote the constructed graph by $\tilde{G} = (\tilde{V}, \tilde{E})$. We also denote the arc set induced by E_0 and $\tilde{E}$ by A_0 and $\tilde{A}$ respectively. For any arc $a = (u, v) \in \tilde{A}$, we write $\overline{a} = (v, u)$, $o(a) = u$ and $t(a) = v$. Remark that $o(\overline{a}) = t(a)$ and $t(\overline{a}) = o(a)$.

The total state space associated with the quantum walk treated here is $\mathbb{C}^{\tilde{A}}$. We define the time evolution operator W on $\mathbb{C}^{\tilde{A}}$ in the matrix form by

$$(W)_{a,b} = \begin{cases} \left(\dfrac{2}{\deg(o(a))} - \delta_{a\bar{b}}\right) & \text{if } o(a) = t(b), \\ 0 & \text{otherwise,} \end{cases}$$

which is so called the Grover walk. Note that the walk becomes “free” on the tails; that is,

$$(W)_{a,b} = \begin{cases} 1 & : o(a) = t(b),\ a \neq \bar{b}, \\ 0 & : \text{otherwise} \end{cases}$$

for any $o(a) \notin V_0$. For simplicity, let us denote $v_j^{(0)}$ by u_j. We set the l^∞-initial state by using a complex value z with $|z| = 1$:

$$\Phi_0(a) = \begin{cases} z^{-\mathrm{dist}(u_j, t(a))}\alpha_j & \text{if } o(a) = v_j^{s+1},\ t(a) = v_j^s,\ s = 0, 1, 2, ...,\ j = 1, 2, ..., r, \\ \\ 0 & \text{otherwise.} \end{cases}$$

Then quantum walkers inflows into the internal graph G_0 at every time step n from the tails. On the other hand, a quantum walker outflows towards the tails from the internal graph.

Let $\Phi_n \in \mathbb{C}^{\tilde{A}}$ be the n-th iteration of the quantum walk such that $\Phi_{n+1} = W\Phi_n$. Since the inflow oscillates with respect to the time step, the total state does not converge in the long time limit. We put $\Phi_n' := z^n \Phi_n$, which satisfies $\Phi_{n+1}' = zW\Phi_n'$. The convergence of Φ_n' is ensured by [14] as follows.

Theorem 3.1 ([14]). $\Phi_\infty' := \lim_{n\to\infty} \Phi_n'$ *exists; that is,* $W\Phi_\infty' = z^{-1}\Phi_\infty'$.

Let us focus on the dynamics restricted to the internal graph. To this end, we define the boundary operator of A_0, $\chi : \mathbb{C}^{\tilde{A}} \to \mathbb{C}^{A_0}$ by,

$$(\chi\tilde{f})(a) = \tilde{f}(a), a \in A_0$$

for any $\tilde{f} \in \mathbb{C}^{\tilde{A}}$. The adjoint $\chi^* : \mathbb{C}^{A_0} \to \mathbb{C}^{\tilde{A}}$ is described by

$$(\chi^* f)(a) = \begin{cases} f(a) & \text{if } a \in A_0, \\ 0 & \text{otherwise} \end{cases}$$

for any $f \in \mathbb{C}^{A_0}$. Remark that $\chi\chi^* : \mathbb{C}^{A_0} \to \mathbb{C}^{A_0}$ is the identity operator on $\mathbb{C}^{A_0}$ and $\chi^*\chi : \mathbb{C}^{\tilde{A}} \to \mathbb{C}^{\tilde{A}}$ is the projection operator on $\mathbb{C}^{\tilde{A}}$ with respect to A_0. Putting $\chi\Phi'_n =: \phi'_n$ and $\chi W \chi^* =: E$, we have

$$\phi'_{n+1} = zE\phi'_n + \rho, \ \phi'_0 = 0, \tag{3.1}$$

where $\rho = \chi W \Phi_0$. The dynamical system given by (3.1) can be also accomplished by the restriction to the internal graph of the following alternating quantum walk for $z = -1$ case: the time evolution operator of the alternating quantum walk $U : \mathbb{C}^{\tilde{A}} \to \mathbb{C}^{\tilde{A}}$ is defined in the matrix form by

$$(U)_{a,b} = \begin{cases} (-1)^{1_{V_0}(o(a))} \left(\dfrac{2}{\deg(o(a))} - \delta_{a\bar{b}} \right) & \text{if } o(a) = t(b), \\ 0 & \text{otherwise}, \end{cases} \tag{3.2}$$

where 1_{V_0} is the characteristic function of V_0. The quantum coin assigned at every vertex in the internal graph is the "signed" Grover matrix. The initial state of the walker is

$$\Psi_0(a) = \begin{cases} \alpha_j & \text{if } o(a) = v_j^{(s+1)},\ t(a) = v_j^{(s)},\ s = 0, 1, 2, ...,\ j = 1, ..., r, \\ \\ 0 & \text{otherwise.} \end{cases} \tag{3.3}$$

In this chapter, we consider $\Psi_{n+1} = U\Psi_n$ instead of Φ_n. Since $\Psi_\infty := \lim_{n\to\infty} \Psi_n$ exists and $U\Psi_\infty = \Psi_\infty$ holds according to [14], we compute its stationary state. In particular, we focus on the following quantities.

Definition 3.2. *Scattering matrix: Let* $\boldsymbol{\alpha} := [\alpha_1, \alpha_2, ..., \alpha_r]^T$, $\boldsymbol{\beta} := [\beta_1, \beta_1, ..., \beta_r]^T$, *where* $\beta_j = \Psi_\infty(a)$ *with* $o(a) = v_j^{(0)}$, $t(a) = v_j^{(1)}$. *The scattering matrix* σ, *which is an* r*-dimensional unitary matrix, is defined by*

$$\boldsymbol{\beta} = \sigma\boldsymbol{\alpha}$$

for any choice of $\boldsymbol{\alpha}$.

The existence of such a unitary matrix is ensured by [7, 8]. If $z = 1$, the scattering matrix gives us only the information of the number of tails because the scattering matrix for $z = 1$ is expressed by $\mathrm{Gr}(r)$ [12]. In this chapter, setting $z = -1$, we obtain the information on the internal graph in Theorem 3.5. We are also interested in the stationary state in the internal graph, especially how many quantum walkers exist; that is, how quantum walkers feel *comfortable* to the graph.

Definition 3.3. *The comfortability of* G_0 *with* $\boldsymbol{\alpha}$ *with* δV *for quantum walker :*

$$\mathcal{E}_{QW}(G_0; \boldsymbol{\alpha}, \delta V) = \frac{1}{2} \sum_{a \in A_0} |\Psi_\infty(a)|^2.$$

We extract some geometric graph structures from these quantities which derive from some quantum effects in Theorem 3.11.

3.2 Scattering matrix

In this section, we obtain the scattering matrix in our model, which gives a characterization of bipartite graphs. To obtain this scattering matrix, we first give the following lemma.

Lemma 3.4. *For a given* $u \in V_0$, $\Psi_\infty(a) - \Psi_\infty(\overline{a})$ *is constant for all* $a \in \tilde{A}$ *with* $o(a) = u$.

Proof. It follows from the dynamics of the walk that, in the stationary state, for $a \in \tilde{A}$ such that $o(a) \in A_0$,

$$\Psi_\infty(a) = -\sum_{b:t(b)=o(a)} \frac{2}{\deg(o(a))}\Psi_\infty(b) + \Psi_\infty(\overline{a}).$$

It follows that

$$\Psi_\infty(a) - \Psi_\infty(\overline{a}) = -\frac{2}{\deg(u)} \sum_{b:t(b)=u} \Psi_\infty(b),\ o(a) = u.$$

Observe that for a given $u \in V_0$, the right hand side of the equation is a constant. $\square$

Now using the above lemma, we obtain the following theorem.

Theorem 3.5. (Scattering on the surface) *Assume the time evolution operator is described by (3.2). For the stationary state Ψ_∞, let $\boldsymbol{\alpha} := [\alpha_1, \alpha_2, ..., \alpha_r]^T$ and $\boldsymbol{\beta} := [\beta_1, \beta_1, ..., \beta_r]^T$, where α_j is the inflow described by (3.3) and β_j is the outflow described by $\beta_j = \Psi_\infty(a)$ with $o(a) = v_j^{(0)}$, $t(a) = v_j^{(1)}$. Then the scattering matrix, which is an r-dimensional unitary matrix; $\boldsymbol{\beta} = \sigma\boldsymbol{\alpha}$, is expressed as follows.*

$$\sigma = \begin{cases} I & : G_0 \text{ is non-bipartite,} \\ \tau & : G_0 \text{ is bipartite.} \end{cases}$$

Here I is the identity matrix and τ is described as follows:

$$\tau = -\begin{bmatrix} I_k & 0 \\ 0 & -I_{r-k} \end{bmatrix} \mathrm{Gr}(r) \begin{bmatrix} I_k & 0 \\ 0 & -I_{r-k} \end{bmatrix}$$

with the computational basis labeled by $\left\{v_1^{(0)}, ..., v_k^{(0)}, v_{k+1}^{(0)}, ..., v_r^{(0)}\right\}$, where $v_1^{(0)}, ..., v_k^{(0)} \in X \cap \delta V$ and $v_{k+1}^{(0)}, ..., v_r^{(0)} \in Y \cap \delta V$. Here X and Y are the partite sets of the underlying bipartite graph.

Proof. By Lemma 3.4, $\Psi_\infty(a) - \Psi_\infty(\overline{a})$ is a constant on $u \in V_0$ such that $o(a) = u$, We denote this value by $\rho(u)$. That is, $\Psi_\infty(a) - \Psi_\infty(\overline{a}) = \rho(u), o(a) = u$. It follows that if $u \sim v$ then $\rho(u) = -\rho(v)$.

Suppose G_0 is non-bipartite. Then there is an odd cycle $C = (u_1, ..., u_{2l-1}), u_i \in V_0$ in G_0. Then we have $\rho(u_1) = -\rho(u_2) = \rho(u_3) = ... = \rho(u_{2l-1}) = -\rho(u_1)$ which implies $\rho(u_1) = 0$. Since G_0 is connected, $\rho(u) = 0$ for any $u \in V_0$. Thus $\Psi_\infty(a) - \Psi_\infty(\overline{a}) = 0$ for any $a \in A_0$ such that $o(a) \in V_0$. In particular $\beta_i = \alpha_i$ for any i. Hence $\boldsymbol{\beta} = \boldsymbol{\alpha}$.

Now suppose G_0 is bipartite with bipartition $V_0 = X \sqcup Y$. Observe that

$$s := \rho(v) \tag{3.4}$$

is constant for all $v \in X$. Then

$$\rho(v) = -s \tag{3.5}$$

for all $v \in Y$. Define

$$\begin{aligned} A_{in}^X &= \left\{a \in \tilde{A} : o(a) \in \tilde{V} \setminus V_0, t(a) \in X\right\}, \\ A_{out}^X &= \left\{a \in \tilde{A} : \overline{a} \in A_{in}^X\right\}, \\ A_{in}^Y &= \left\{a \in \tilde{A} : o(a) \in \tilde{V} \setminus V_0, t(a) \in Y\right\}, \\ A_{out}^Y &= \left\{a \in \tilde{A} : \overline{a} \in A_{in}^Y\right\}. \end{aligned}$$

Then by applying the time evolution operator once, we get

$$U\left(\Psi_\infty|_{A_{in}^X} + \Psi_\infty|_{A_{in}^Y} + \Psi_\infty|_{A_0}\right) = \Psi_\infty|_{A_{out}^X} + \Psi_\infty|_{A_{out}^Y} + \Psi_\infty|_{A_0}.$$

By taking the squared norm, we get

$$\left\|\Psi_\infty|_{A_{in}^X}\right\|^2 + \left\|\Psi_\infty|_{A_{in}^Y}\right\|^2 + \|\Psi_\infty|_{A_0}\|^2 = \left\|\Psi_\infty|_{A_{out}^X}\right\|^2 + \left\|\Psi_\infty|_{A_{out}^Y}\right\|^2 + \|\Psi_\infty|_{A_0}\|^2.$$

It follows from (3.4) and (3.5) that

$$\begin{aligned}\left\|\Psi_\infty|_{A_{in}^X}\right\|^2+\left\|\Psi_\infty|_{A_{in}^Y}\right\|^2 &= \left\|s1_{A_{in}^X}+S\Psi_\infty|_{A_{in}^X}\right\|^2+\left\|-s1_{A_{in}^Y}+S\Psi_\infty|_{A_{in}^Y}\right\|^2 \\ &= s^2|X\cap\delta V|+2s\sum_{a\in A_{in}^X}\Psi_\infty(a)+\left\|\Psi_\infty|_{A_{in}^X}\right\|^2 \\ &\quad + s^2|Y\cap\delta V|-2s\sum_{a\in A_{in}^Y}\Psi_\infty(a)+\left\|\Psi_\infty|_{A_{in}^Y}\right\|^2.\end{aligned}$$

Here S is the shift operator: $S\delta_a=\delta_{\bar a}$ for any $a\in\tilde A$. Hence if $s\neq 0$,

$$s=-\frac{2}{|\delta V|}\left(\sum_{a\in A_{in}^X}\Psi_\infty(a)-\sum_{a\in A_{in}^Y}\Psi_\infty(a)\right). \tag{3.6}$$

Then it follows that

$$\beta_i=\alpha_i-\frac{2}{|\delta V|}\left(\sum_{a\in A_{in}^X}\Psi_\infty(a)-\sum_{a\in A_{in}^Y}\Psi_\infty(a)\right),$$

where $\beta_i=\Psi_\infty(a)$ for some $a\in A_{out}^X$ and

$$\beta_i=\alpha_i-\frac{2}{|\delta V|}\left(\sum_{a\in A_{in}^Y}\Psi_\infty(a)-\sum_{a\in A_{in}^X}\Psi_\infty(a)\right),$$

where $\beta_i=\Psi_\infty(a)$ for some $a\in A_{out}^Y$. Hence $\boldsymbol{\beta}=\tau\boldsymbol{\alpha}$ where

$$\tau=\left(\begin{array}{ccc|c} -\frac{2}{|\delta V|}+1 & -\frac{2}{|\delta V|} & \cdots & \\ -\frac{2}{|\delta V|} & -\frac{2}{|\delta V|}+1 & \cdots & \frac{2}{|\delta V|} \\ \vdots & & & \\ \hline & & & \begin{array}{ccc} -\frac{2}{|\delta V|}+1 & -\frac{2}{|\delta V|} & \cdots \\ -\frac{2}{|\delta V|} & -\frac{2}{|\delta V|}+1 & \cdots \\ \vdots & & \end{array} \\ & \frac{2}{|\delta V|} & & \end{array}\right).$$

It is clear that, to satisfy the condition $s\neq 0$, we must have $\sum_{a\in A_{in}^Y}\Psi_\infty(a)\neq\sum_{a\in A_{in}^X}\Psi_\infty(a)$. Now let us see that $s=0$ if and only if $\kappa_X=\kappa_Y$, where $\kappa_X=\sum_{a\in A_{in}^X}\Psi_\infty(a)$ and $\kappa_Y=\sum_{a\in A_{in}^Y}\Psi_\infty(a)$.

By Lemma 3.4 we have, $s=0$ if and only if

$$\Psi_\infty(a)=\Psi_\infty(\overline{a}),\ a \text{ with } o(a)\in A_0$$

and

$$\sum_{b:t(b)=u}\Psi_\infty(b)=0,\ u\in V_0.$$

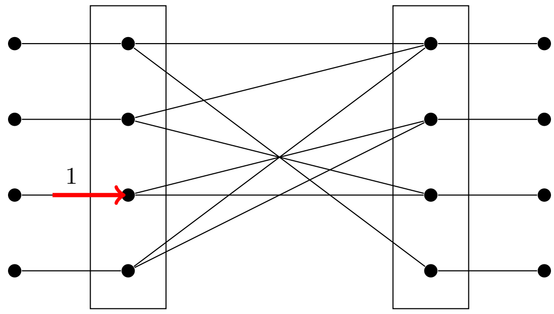

Figure 3.1: Example of the inflow of $s \neq 0$.

Thus we have

$$\begin{aligned} 0 &= \sum_{a:t(a)\in Y} \Psi_\infty(a) \\ &= \sum_{a:\, t(a)\in Y,\, o(a)\in X} \Psi_\infty(a) + \kappa_Y \\ &= \sum_{a:\in o(a)\in X,\, t(a)\in Y} \Psi_\infty(a) + \kappa_Y \\ &= \sum_{a:o(a)\in X} \Psi_\infty(a) - \kappa_X + \kappa_Y \\ &= -\kappa_X + \kappa_Y, \end{aligned}$$

which implies $\kappa_X = \kappa_Y$ if $s = 0$.

If $\boldsymbol{\alpha}$ satisfies $\kappa_X = \kappa_Y$, then $s = 0$ and the same argument as in the case where G_0 is non-bipartite is valid; $\boldsymbol{\beta} = \boldsymbol{\alpha}$ holds. It is easy to check that $\boldsymbol{\beta} = \tau\boldsymbol{\alpha}$ holds for τ defined above. $\square$

Remark. *If we set the inflow to a bipartite graph with the partite sets X and Y so that total inflow to the partite set X coincides with that to the partite set Y, the perfect reflecting happens. This means that we can not detect the bipartiteness of graph with such an initial state. These inputs vectors are described by eigenvectors of the scattering matrix τ with the eigenvalue 1.*

3.3 Kirchhoff and pseudo-Kirchhoff laws

In this section we will see that the stationary state can represent a kind of current function [12, 14] on the underlying bipartite and non-bipartite graphs.

Bipartite case

First, we will introduce a current function induced by the stationary state Ψ_∞ on a bipartite graph. Let G_0 be a bipartite graph with bipartition $V_0 = X \sqcup Y$. Define the function $f(\cdot)$ such that

$$f(a) = \begin{cases} 0 & \text{if } t(a) \in X, \\ \\ 1 & \text{if } t(a) \in Y. \end{cases}$$

Then by Lemma 3.4, it follows that the measure $\frac{1}{2}\left((-1)^{f(a)}\Psi_\infty(a) + (-1)^{f(\overline{a})}\Psi_\infty(\overline{a})\right)$ is a constant for any $a \in A_0$. We denote this constant by ρ. Then the following theorem holds.

Theorem 3.6. *Let the setting be the same as the above and define $j(a) = (-1)^{f(a)}\Psi_\infty(a) - \rho$. Then $j(\cdot)$ satisfies the Kirchhoff's current and voltage laws:*

1. *(Kirchhoff current law) For any $u \in \tilde{V}$ and $a \in \tilde{A}$,*

$$\sum_{b \in \tilde{A}: t(b)=u} j(b) = 0; \ j(a) + j(\overline{a}) = 0.$$

2. *(Kirchhoff voltage law) For any cycle $c = (a_1, ..., a_s)$ with $t(a_1) = o(a_2), ..., t(a_{s-1}) = o(a_s), t(a_s) = o(a_1)$ in G_0, it holds*

$$\sum_{k=1}^{s} j(a_k) = 0.$$

Proof. We can rewrite the expression in Lemma 3.4 as

$$\frac{1}{2}\left((-1)^{f(a)}\Psi_\infty(a) + (-1)^{f(\overline{a})}\Psi_\infty(\overline{a})\right) = \frac{1}{\deg(u)} \sum_{b: t(b)=u} (-1)^{f(b)}\Psi_\infty(b), \ o(a) = u,$$

in which the right hand side is a measure on the vertex u, denoted by $\rho(u)$. Then it follows that if $u \sim v$ then $\rho(u) = \rho(v)$. Since G_0 is connected, it follows that $\rho(u)$ is a constant for all $u \in V_0$, which is denoted by ρ. Summarizing the above, we have

$$\frac{1}{\deg(u)} \sum_{b: t(b)=u} (-1)^{f(b)}\Psi_\infty(b) = \rho, u \in V_0. \tag{3.7}$$

Then from (3.6) we can express

$$\rho = \frac{1}{|\delta V|}\left(\sum_{a \in A_{in}^X} \Psi_\infty(a) - \sum_{a \in A_{in}^Y} \Psi_\infty(a)\right).$$

Equation (3.7) implies

$$\sum_{a: t(a)=u} j(a) = \sum_{a: t(a)=u} (-1)^{f(a)}\Psi_\infty(a) - \rho \deg(u) = 0, \ u \in V_0.$$

Also we have

$$j(a) + j(\overline{a}) = (-1)^{f(a)}\Psi_\infty(a) + (-1)^{f(\overline{a})}\Psi_\infty(\overline{a}) - 2\rho = 0, \ a \in A_0.$$

Now suppose $C = (a_1, ..., a_{2l}), a_i \in A_0$ is an even cycle in G_0. Assume that $o(a_1) \in X$. Define φ such that

$$\varphi(a) = \begin{cases} 1 & \text{if } a = a_{2k+1} \text{ or } \overline{a}_{2k+1}, \\ -1 & \text{if } a = a_{2k} \text{ or } \overline{a}_{2k}, \\ 0 & \text{otherwise.} \end{cases}$$

Let $\psi_\infty := \chi^* \Psi_\infty$. Since φ is a centered eigenvector of $\chi U \chi^*$ whose eigenvalue is -1, by [14, Lemmas 3.4 and 3.5] we have $\psi_\infty \perp \varphi$ and it follows that

$$\begin{aligned} 0 &= \langle \psi_\infty | \varphi \rangle \\ &= \sum_{a \in A_0} \psi_\infty(a)\varphi(a) \\ &= \sum_{k=1}^{l} \left[[\psi_\infty(a_{2k-1}) + \psi_\infty(\overline{a}_{2k-1})] - [\psi_\infty(a_{2k-1}) + \psi_\infty(\overline{a}_{2k-1})]\right] \\ &= \sum_{k=1}^{l} \left[(-1)^{f(a_{2k-1})}\left(j(a_{2k-1}) - j(\overline{a}_{2k-1})\right) - (-1)^{f(a_{2k})}\left(j(a_{2k}) - j(\overline{a}_{2k})\right)\right] \\ &= \sum_{k=1}^{2l} \left[j(a_k) - j(\overline{a}_k)\right]. \end{aligned}$$

Since $j(a) + j(\overline{a}) = 0$, it follows that

$$\sum_{k=1}^{s} j(a_k) = 0.$$

$\square$

Non-bipartite case

Next let us investigate the property of ψ_∞ in the non-bipartite case. We can see that the stationary state itself has similar properties to the electrical current flow as follows.

Theorem 3.7. *Let $\psi_\infty \in \mathbb{C}^{A_0}$ be the stationary state on the non-bipartite graph. Then ϕ_∞ satisfies the following properties:*

1. *(Pseudo-Kirchhoff current law) For each $u \in V_0$ and $a \in A_0$,*

$$\sum_{t(a)=u} \psi_\infty(a) = 0, \ \psi_\infty(a) = \psi_\infty(\bar{a}).$$

2. *(Pseudo-Kirchhoff voltage law) For any even closed walk $(e_1, \ldots, e_{2s})$ such that $t(e_1) = o(e_2), \ldots, t(e_{2s-1}) = o(e_{2s})$ and $t(e_{2s}) = o(e_1)$,*

$$\sum_{k=1}^{2s} (-1)^k \psi_\infty(e_k) = 0.$$

Proof. The proof of the first part is obtained from the proof of Theorem 3.5. To prove the second part, for an even closed walk $(e_1, \ldots, e_{2s})$ such that $t(e_1) = o(e_2), \ldots, t(e_{2s-1}) = o(e_{2s})$ and $t(e_{2s}) = o(e_1)$, define the function ϕ by

$$\phi(a) = \begin{cases} (-1)^k & \text{if } a = e_k \text{ or } a = \overline{e_k}, \\ \\ 0 & \text{otherwise.} \end{cases}$$

Note that in the case when the arcs in the walk overlap, then $\phi(a)$ is set to be the sum of all such values defined above, on the corresponding arcs. Then it is easy to check that ϕ is an eigenvector of U with the eigenvalue -1. By the proof of the convergence of Ψ_∞, it follows that $\langle \phi, \Psi_\infty \rangle = 0$ which gives the desired conclusion. $\square$

3.4 Laplacian and signless Laplacian

We have seen that the stationary state has the properties of current function or pseudo-current function in $\mathbb{C}^{A_0}$. Then it is natural to determine the potential function in $\mathbb{C}^{V_0}$ with respect to the current. In this subsection, we characterize the potential function using the Laplacian and the signless Laplacian for the cases of bipartite and non-bipartite graphs, respectively.

Bipartite case

Let M be the adjacency matrix and D be the degree matrix of G_0. The Laplacian matrix of G_0 is denoted by $L = D - M$. Using the Laplacian matrix with the Poisson equation, we can characterise the current function $j(\cdot)$ on A_0 in terms of a potential function on V_0 ([3] and [4]) in which exists under the Kirchhoff current and voltage laws.

Theorem 3.8 (see e.g., [3, 4])**.** *Let the setting be the same as in Theorem 3.6. Let G_0 be a bipartite graph and L be the Laplacian matrix of G_0. Then there exists a potential function $\phi \in \mathbb{C}^{V_0}$ such that $j(a) = \phi(o(a)) - \phi(t(a))$. Here ϕ satisfies the following equation.*

$$L\phi = -q,$$

where $q(u) = \sum_{a \in \tilde{A} \setminus A_0 : t(a) = u} j(a), \ u \in V_0.$

Proof. Let $V_0 = \{v_1, ..., v_n\}$. Denote the incidence mapping by $B : \mathbb{C}^{A_0} \to \mathbb{C}^{V_0}$ which satisfies

$$(B\psi)(v_i) = \sum_{j=1}^{m} b_{ij}\psi(a_j), 1 \le i \le n$$

where $m = |A_0|$ and

$$b_{ij} = \begin{cases} 1 & \text{if } t(a_j) = v_i, \\ -1 & \text{if } o(a_j) = v_i, \\ 0 & \text{otherwise.} \end{cases}$$

Then we have

$$(B\psi)(v) = \sum_{a \in A_0 : t(a) = v} \psi(a) - \sum_{a \in A_0 : o(a) = v} \psi(a), v \in V_0.$$

The adjoint operator $B^* : \mathbb{C}^{V_0} \to \mathbb{C}^{A_0}$ is given by

$$(B^* f)(a) = f(t(a)) - f(o(a)).$$

Then we have BB^* in terms of the Laplacian matrix L

$$BB^* = 2(D - M) = 2L.$$

If the potential function is $\phi \in \mathbb{C}^{V_0}$ and the conductance along each arc is assumed to be 1, by the Ohm's law,

$$\begin{aligned} j(a) &= \phi(o(a)) - \phi(t(a)) \\ &= -(B^*\phi)(a). \end{aligned}$$

Now we can state the latter part of the Kirchhoff's current law as follows.

$$j(a) = \phi(o(a)) - \phi(t(a)) = \phi(t(\overline{a})) - \phi(o(\overline{a})) = -j(\overline{a}), a \in A_0.$$

And it follows that

$$\begin{aligned} \sum_{a \in \tilde{A} : o(a) = u} j(a) &= - \sum_{a \in \tilde{A} : o(a) = u} j(\overline{a}) \\ &= - \sum_{a \in \tilde{A} : t(a) = u} j(a) \end{aligned}$$

which implies

$$\sum_{a \in \tilde{A} : t(a) = u} j(a) = 0, u \in V_0.$$

Now we can denote the first part of the Kirchhoff's current law in terms of the incident matrix as follows.

$$\sum_{a \in A_0 : t(a) = u} j(a) + \sum_{a \in \tilde{A} \setminus A_0 : t(a) = u} j(a) - \sum_{a \in A_0 : o(a) = u} j(a) - \sum_{a \in \tilde{A} \setminus A_0 : o(a) = u} j(a) = 0$$

And it follows that

$$(Bj)(u) = -2 \sum_{a \in \tilde{A} \setminus A_0 : t(a) = u} j(a).$$

This gives an analogy of the equation given in [3] as

$$Bj = -2q$$

where $q(u) = \sum_{a \in \tilde{A} \setminus A_0 : t(a) = u} j(a), u \in V_0$. In other words,

$$L\phi = -q.$$

Moreover, for any cycle $c = (a_1, ..., a_s)$ with $t(a_1) = o(a_2), ..., t(a_{s-1}) = o(a_s), t(a_s) = o(a_1)$ in G_0, taking the sum of $j(a_i) = \phi(o(a_i)) - \phi(t(a_i))$ over the cycle, the Kirchhoff's voltage law satisfies. $\square$

Here we should remark that $q \in (\ker(L))^{\perp}$: actually we have

$$0 = \sum_{a \in A : t(a) \in V_0} j(a) \equiv \sum_{a \in A \setminus A_0 : t(a) \in V_0} j(a) = \sum_{v \in V_0} q(v)\mathbf{1}(v),$$

where $\mathbf{1}(\cdot)$ is the constant function whose value is 1 and $\ker(L) = \{c\mathbf{1} : c \in \mathbb{C}\}$.

Non-bipartite case
When the underlying graph is non-bipartite, the following two properties hold for the stationary sate Ψ_∞ by Theorem 3.7:

$$\Psi_\infty(a) = \Psi_\infty(\overline{a}), \text{ for any } a \in \tilde{A}, o(a) \in V_0; \tag{3.8}$$

$$\sum_{a \in \tilde{A} : t(a) = u} \Psi_\infty(a) = 0, \text{ for any } u \in V_0. \tag{3.9}$$

As an analogy to the current function in the bipartite case, we represent these properties in terms of the non-oriented incidence matrix and the *signless* Laplacian matrix in the following theorem. Here the signless Laplacian matrix of G_0 is denoted by $Q = M + D$.

Theorem 3.9. *Let Ψ_∞ be the stationary state of quantum walk such that $\Psi_\infty(a) = \lim_{n\to\infty}(U^n\Psi_0)(a)$ for any $a \in \tilde{A}$. Let G_0 be a non-bipartite graph and Q be the signless Laplacian matrix of G_0. Then there uniquely exists $\phi \in \mathbb{C}^{V_0}$ such that $\Psi_\infty(a) = \phi(o(a)) + \phi(t(a))$ for any $a \in A_0$. Here ϕ satisfies the following equation.*

$$Q\phi = -q$$

where $q(u) = \sum_{a \in \tilde{A} \setminus A_0 : t(a) = u} \Psi_\infty(a), \ u \in V_0$.

Proof. Denote the non-oriented incidence matrix on the set of arcs by $\tilde{C} : \mathbb{C}^{A_0} \to \mathbb{C}^{V_0}$ which satisfies

$$(\tilde{C}\psi)(v_i) = \sum_{j=1}^{m} c_{ij}\psi(a_j), \ 1 \le i \le n,$$

where $m = |A_0|$ and

$$c_{ij} = \begin{cases} 1 & \text{if } t(a_j) = v_i \text{ or } o(a_j) = v_i, \\ 0 & \text{otherwise.} \end{cases}$$

Then we have

$$(\tilde{C}\psi)(v) = \sum_{a \in A_0 : t(a) = v} \psi(a) + \sum_{a \in A_0 : o(a) = v} \psi(a), \ v \in V_0.$$

The adjoint operator $\tilde{C}^* : \mathbb{C}^{V_0} \to \mathbb{C}^{A_0}$ is given by

$$(\tilde{C}^* f)(a) = f(t(a)) + f(o(a)).$$

Then we have $\tilde{C}\tilde{C}^*$ in terms of the signless Laplacian matrix Q

$$\tilde{C}\tilde{C}^* = 2(D + M) = 2Q.$$

Let $\psi_\infty = \chi^*\Psi_\infty$. Now let us see that if there exists a potential function $\phi \in \mathbb{C}^{V_0}$ such that $\psi_\infty(a) = (\tilde{C}^*\phi)(a)$ for any $a \in A_0$, then ϕ must satisfy

$$Q\phi = -q.$$

Remark that for any $a \in A_0$

$$\psi_\infty(a) = (\tilde{C}^*\phi)(a) = \phi(t(a)) + \phi(o(a)) = \phi(t(\overline{a})) + \phi(o(\overline{a})) = (\tilde{C}^*\phi)(\overline{a}) = \psi_\infty(\overline{a})$$

and hence the first property of (3.8) can be easily confirmed. We have, by the property (3.8),

$$\sum_{a\in\tilde{A}:o(a)=u}\Psi_\infty(a)=\sum_{a\in\tilde{A}:o(a)=u}\Psi_\infty(\overline{a})$$
$$=\sum_{a\in\tilde{A}:t(a)=u}\Psi_\infty(a),$$

and by the property (3.9),

$$\sum_{a\in\tilde{A}:t(a)=u}\Psi_\infty(a)+\sum_{a\in\tilde{A}:o(a)=u}\Psi_\infty(a)=0,\ u\in V_0.$$

Let us divide the summation in the above equation by

$$\sum_{a\in A_0:t(a)=u}\Psi_\infty(a)+\sum_{a\in\tilde{A}\setminus A_0:t(a)=u}\Psi_\infty(a)+\sum_{a\in A_0:o(a)=u}\Psi_\infty(a)+\sum_{a\in\tilde{A}\setminus A_0:o(a)=u}\Psi_\infty(a)=0.$$

Then it follows that

$$(\tilde{C}\psi_\infty)(u)=-2\sum_{a\in\tilde{A}\setminus A_0:t(a)=u}\Psi_\infty(a).$$

which implies

$$Q\phi=\frac{1}{2}\tilde{C}\tilde{C}^*\phi=-q,$$

where $q(u)=\sum_{a\in\tilde{A}\setminus A_0:t(a)=u}\Psi_\infty(a), u\in V_0$. Although the existence of the potential function ϕ is ensured by the pseudo-Kirchhoff voltage law in Theorem 3.7, we prove here directly as follows. To show the existence of ϕ, it is enough to show that

$$\psi_\infty\in\mathrm{Range}(\tilde{C}^*)=\ker(\tilde{C})^\perp.$$

Let us see that

$$\ker(\tilde{C})=(\ker(d)\cap\mathcal{H}_+)\oplus\mathcal{H}_-, \tag{3.10}$$

where $\mathcal{H}_+=\left\{\psi\in\mathbb{C}^{A_0}:\psi(a)=\psi(\overline{a})\text{ for any }a\in A_0\right\}$, $\mathcal{H}_-=\left\{\psi\in\mathbb{C}^{A_0}:\psi(a)=-\psi(\overline{a})\text{ for any }a\in A_0\right\}$ and

$$(d\varphi)(u)=\frac{1}{\sqrt{\deg_{G_0}(u)}}\sum_{a\in A_0:t(a)=u}\varphi(a).$$

Note that $\mathcal{H}_+\oplus\mathcal{H}_-=\mathbb{C}^{A_0}$ and $\mathcal{H}_+=\ker(1-S_0)$, $\mathcal{H}_-=\ker(1+S_0)$, where S_0 is the shift operator on $\mathbb{C}^{A_0}$ such that $S_0\delta_a=\delta_{\overline{a}}$ for any $a\in A_0$. The operator $\tilde{C}$ can be rewritten by

$$(\tilde{C}\psi)(u)=\sqrt{\deg_{G_0}(u)}\left((d\psi)(u)+(dS_0\psi)(u)\right).$$

Then we have

$$\ker\tilde{C}=\ker(d(1+S_0)),$$

which implies (3.10). By [14] it follows that

$$\psi_\infty\in(\ker(d)\cap\mathcal{H}_+)^\perp.$$

Since $\psi_\infty(\bar{a})=\psi_\infty(a)$, then $\psi_\infty\in\mathcal{H}_+=\mathcal{H}_-^\perp$. Therefore $\psi_\infty\in\ker(\tilde{C})^\perp=\mathrm{Range}(\tilde{C}^*)$.

Furthermore, since G_0 is non-bipartite, the least eigenvalue of Q is positive (cf. [6]) and hence Q is invertible. This completes the proof of the existence and the uniqueness of ϕ. □

3.5 Comfortability

We have seen that relations between stationary state and the (signless-)Laplacian, which contains information of the geometry of the graph. Let us express the comfortability in terms of some graph geometrical properties.

Definition 3.10. (Important graph factors) *Let $\chi_1(G_0)$ be the number of spanning trees of G_0 and $\chi_2(G_0; u_1, u_n)$ be the number of spanning forests of G_0 with exactly two components, one containing u_1 and the other containing u_n. Here the isolate vertex is regarded as a tree.*

Let $\mathcal{C}_o$ be the set of spanning subgraphs of G_0 all of whose components are odd unicyclic graphs and let $\mathcal{TC}_o$ be the set of spanning subgraphs of G_0 whose one component is a tree containing the vertex u_1 and remaining components are odd unicyclic graphs, which are possibly empty. Note that $\mathcal{TC}_o$ contains the spanning trees of G_0 as well. See Figure 3.2.

Now define the functions ι_1 and ι_2 by

$$\iota_1(G_0) = \sum_{H \in \mathcal{C}_o} 4^{\omega(H)}$$

and

$$\iota_2(G_0; u_1) = \sum_{H \in \mathcal{TC}_o} 4^{\omega(H)-1},$$

where $\omega(H)$ is the number of components in H.

Then with the above notations, we have the following theorem.

Theorem 3.11. (Comfortability in the interior) *Assume the number of tails is 2, and the inflow $\boldsymbol{\alpha} = (\alpha_1, \alpha_2) = (1, 0)$ at u_1 and u_n, respectively. Then the comfortability of the quantum walk (3.2) is given by*

$$\mathcal{E}_{QW}(G_0; u_1, u_n) = \begin{cases} \dfrac{1}{4}\left(\dfrac{\chi_2(G_0; u_1, u_n)}{\chi_1(G_0)} + |E_0|\right) & \text{if } G_0 \text{ is bipartite,} \\ \\ \dfrac{\iota_2(G_0; u_1)}{\iota_1(G_0)} & \text{if } G_0 \text{ is non-bipartite.} \end{cases}$$

Then we can determine how much quantum walker feels *comfortable* to the given graph by listing up the spanning subgraphs in Definition 3.10 of this graph. We will demonstrate it for the graphs with four vertices in the next section.

Proof. **Bipartite case**
Now we introduce the energy of the electric circuit $\mathcal{E}_{EC}(G_0)$ which is given by,

$$\mathcal{E}_{EC}(G_0) = \frac{1}{2}\|j\|^2 = \frac{1}{2}\sum_{a \in A_0} |j(a)|^2.$$

To give the next proposition, we prepare the following notion. Note that the Laplacian matrix L is singular and hence ϕ is not determined uniquely. We impose the ground condition $\phi(n) = 0$ which reduces the equation in Theorem 3.8 to $L^{(n)}\phi^{(n)} = -q^{(n)}$, where $L^{(n)}$ is the matrix obtained by removing the n-th row and the n-th column of the Laplacian matrix, $\phi^{(n)}$ and $q^{(n)}$ are the vectors obtained by removing the n-th element from ϕ and q respectively. Here, $\det(L^{(n)})$ is the number of spanning trees of G_0 (see [3]), and hence non-zero. So $\phi^{(n)}$ is determined uniquely by $\phi^{(n)} = -(L^{(n)})^{-1}q^{(n)}$. More over, we denote by B and $\tilde{B}$, the usual incidence matrix and the non-oriented incidence matrix on the set of edges respectively. More precisely, we fix an orientation of each $e \in E_0$ and denote it by $\vec{E}_0$:

$$A_0 = \vec{E}_0 \cup \overline{(\vec{E}_0)},$$

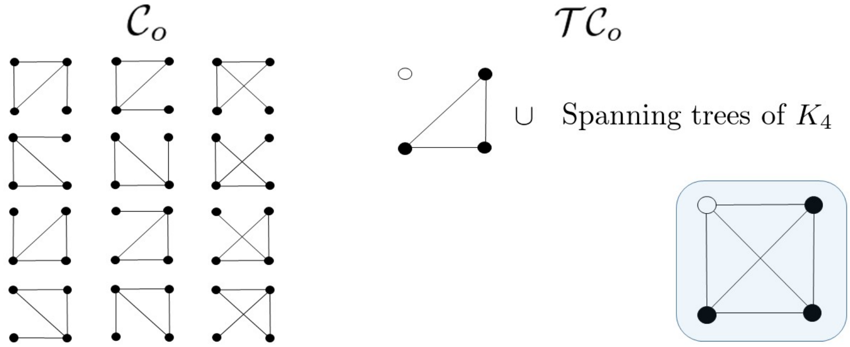

Figure 3.2: $\mathcal{C}_o$-factor and $\mathcal{TC}_o$-factor of K_4: The white colored vertex in the complete graph K_4 corresponds to u_1. The left figure depicts the list of the family of odd unicyclic factor of K_4 and the right figure depicts the list of the $\mathcal{TC}_o$-factor of K_4. Note that the isolated vertex is regards as a tree and the family of the spanning tree is included in $\mathcal{TC}_o$.

where $\overline{(\vec{E}_0)} = \{a \in A_0 \mid \bar{a} \in \vec{E}_0\}$. Then $B : \mathbb{C}^{\vec{E}_0} \to \mathbb{C}^{V_0}$ is denoted by

$$(B\psi)(u) = \sum_{t(a)=u} \psi(a) - \sum_{o(a)=u} \psi(a);$$

then its adjoint is expressed by

$$(B^* f)(a) = f(t(a)) - f(o(a)).$$

The non-oriented incidence matrix $\tilde{B} : \mathbb{C}^{\vec{E}_0} \to \mathbb{C}^{V_0}$ is denoted by

$$(\tilde{B}\psi)(u) = \sum_{t(a)=u} \psi(a) + \sum_{o(a)=u} \psi(a);$$

then its adjoint is expressed by

$$(\tilde{B}^* f)(a) = f(t(a)) + f(o(a)).$$

Now we give the following proposition.

Proposition 3.12. *The electrical energy of the circuit is given by*

$$\varepsilon_{EC}(G_0) = \frac{1}{\det(L^{(n)})} \sum_{i,j=1}^{n-1} (-1)^{i+j} q^{(n)}(i) q^{(n)}(j) \sum_{\substack{H \subset G_0 \\ |E(H)|=n-2}} \det(B_H^{(n,j)}) \det((B_H^{(n,i)})^*),$$

where $B_H^{(n,j)}$ is the matrix obtained by choosing the columns corresponding to the edges in H and removing the j-th and n-th rows in the oriented incidence matrix of G_0.

Proof. By definition, we can write the electrical energy in terms of the Laplacian matrix as follows.

$$\begin{aligned}\varepsilon_{EC}(G_0) &= \frac{1}{2}\|j\|^2 = \langle B^*\phi, B^*\phi\rangle = \langle \phi, L\phi\rangle = -\langle \phi, q\rangle = -\left\langle \phi^{(n)}, q^{(n)}\right\rangle = \left\langle (L^{(n)})^{-1} q^{(n)}, q^{(n)}\right\rangle \\ &= \sum_{i=1}^{n-1} q^{(n)}(i)((L^{(n)})^{-1} q^{(n)})(i).\end{aligned}$$

By Cramer's rule, we get,

$$\varepsilon_{EC}(G_0) = \frac{1}{\det(L^{(n)})}\sum_{i=1}^{n-1} q^{(n)}(i)\det(L_i^{(n)}),$$

where $L_i^{(n)}$ is the matrix obtained by replacing the i-th column of $L^{(n)}$ by $q^{(n)}$. Now by expanding along the i-th column, we get

$$\varepsilon_{EC}(G_0) = \frac{1}{\det(L^{(n)})}\sum_{i,j=1}^{n-1} q^{(n)}(i)q^{(n)}(j)\det(L_{(j,i)}^{(n)}),$$

where $L_{(j,i)}^{(n)}$ is the matrix obtained by removing the j-th row and the i-th column from $L^{(n)}$. Note that $L_{(j,i)}^{(n)} = B^{(j,n)}(B^{(i,n)})^*$ and hence

$$\varepsilon_{EC}(G_0) = \frac{1}{\det(L^{(n)})}\sum_{i,j=1}^{n-1} q^{(n)}(i)q^{(n)}(j)\det(B^{(j,n)}(B^{(i,n)})^*),$$

where $B^{(j,n)}$ is the matrix obtained by removing the j-th and the n-th rows from B. Now by Binet-Cauchy theorem (see [6]), it follows that

$$\varepsilon_{EC}(G_0) = \frac{1}{\det(L^{(n)})}\sum_{i,j=1}^{n-1} (-1)^{i+j}q^{(n)}(i)q^{(n)}(j)\sum_{\substack{H\subset G_0\\|E(H)|=n-2}} \det(B_H^{(n,j)})\det((B_H^{(n,i)})^*),$$

where $B_H^{(n,j)}$ is the matrix obtained by choosing the columns corresponding to the edges in H from $B^{(j,n)}$. $\square$

Now we apply Proposition 3.12. Observing that $\rho = 1/2$, $q^{(n)}(1) = 1-\rho = 1/2$ and $q^{(n)}(i) = 0$ $(i = 2,\dots,n-1)$ in our setting of Theorem 3.11 and applying Proposition 3.12 to our setting, we get

$$\varepsilon_{EC}(G_0) = \frac{1}{4}\frac{1}{\det(L^{(n)})}\sum_{\substack{H\subset G_0\\|E(H)|=n-2}} \left(\det(B_H^{(n,1)})\right)^2.$$

Focusing on the linear dependence on the column vectors of the incidence matrix of the spanning subgraph $H \subset G_0$, we obtain the following:

1. If H contains a cycle, then $\det(B_H^{(n,1)}) = 0$;

2. If H contains a connected component including both u_1 and u_n, then $\det(B_H^{(n,1)}) = 0$.

Hence, it implies that if $\det(B_H^{(n,1)}) \neq 0$, then H is a spanning forest which contains exactly two components, one containing u_1 and the other one containing u_n. On the other hand, if H is a spanning forest which contains exactly two components, one containing u_1 and the other one containing u_n, $B_H^{(n,1)}$ is of the form

$$B_H^{(n,1)} = \left(\begin{array}{c|c} B_{T_1} & 0 \\ \hline 0 & B_{T_2}\end{array}\right)$$

for the trees T_1 and T_2 in the forest which are the spanning trees of the two components of the forest. Now by [3], $\det(B_{T_1}) = \det(B_{T_2}) = \pm 1$ and hence $\left(\det(B_H^{(n,1)})\right)^2 = 1$. Thus, $\left(\det(B_H^{(n,1)})\right)^2 = 1$ if and only if H is a spanning forest which contains exactly two components, one containing u_1 and the other one containing u_n. Hence it follows that

$$\varepsilon_{EC}(G_0) = \frac{\chi_2(G_0; u_1, u_n)}{\chi_1(G_0)}.$$

Let G_0 be a bipartite graph. Then

$$\begin{aligned}\varepsilon_{QW} &= \frac{1}{2}\sum_{a\in A_0}|\Psi_\infty(a)|^2 = \frac{1}{2}\sum_{a\in A_0}|j(a)+\rho|^2 = \frac{1}{2}\sum_{a\in A_0}j(a)^2 + \rho\sum_{a\in A_0}j(a) + \rho^2|E_0| \\ &= \varepsilon_{EC}(G_0) + \rho^2|E_0|. \end{aligned} \tag{3.11}$$

Note that in our setting with only two tails, we have $\rho^2 = \frac{1}{4}$, which leads to the formula in the theorem. □

Non-bipartite case

Now let G_0 be non-bipartite. Then we have $\psi_\infty(e) = \psi_\infty(\bar{e}) = (\tilde{B}^*\phi)(e)$ for any $e \in \vec{E}_0$ and $Q\phi = -q$. Now since G_0 is non-bipartite, it follows that Q is invertible (for example, see [6, Theorem 7.8.1]) and hence $\phi = -Q^{-1}q$. By a similar argument, it follows that

$$\varepsilon_{QW}(G_0) = \frac{1}{2}\sum_{a\in A_0}|\Psi_\infty(a)|^2 = \frac{1}{2}\langle\psi_\infty,\psi_\infty\rangle = \left\langle \tilde{B}^*\phi, \tilde{B}^*\phi\right\rangle = \langle\phi, Q\phi\rangle = \left\langle Q^{-1}q, q\right\rangle.$$

By using the Cramer's rule and the Binet-Cauchy theorem, we can derive a similar expression for the non-bipartite graphs as follows:

Proposition 3.13. *Let G_0 be a non-bipartite graph with an arbitrary choice of u_1 and u_n. Then we have*

$$\varepsilon_{QW}(G_0) = \frac{1}{det(Q)}\sum_{i,j=1}^{n}(-1)^{i+j}q(i)q(j)\sum_{\substack{H\subset G_0\\ |E(H)|=n-1}} det(\tilde{B}_H^{(i)})det(\tilde{B}_H^{(j)}),$$

where $\tilde{B}_H^{(j)}$ is the matrix obtained by choosing the columns corresponding to the edges in H and removing the j-th row from $\tilde{B}$.

Observing that $q(j) = \delta_1(j)$ in our setting and applying Proposition 3.13, then we have

$$\varepsilon_{QW}(G_0) = \frac{1}{\det(Q)}\sum_{\substack{H\subset G_0\\ |E(H)|=n-1}}\left(\det(\tilde{B}_H^{(1)})\right)^2.$$

Focusing on the linear dependence on the column vectors of the incidence matrix of the spanning subgraph $H \subset G \setminus \{u_1\}$, we obtain the following:

1. If H has an even cycle, then $\det(\tilde{B}_H^{(1)}) = 0$;
2. If H has a connected component having at least two odd cycles, then $\det(\tilde{B}_H^{(1)}) = 0$;
3. If H has a connected component having an odd cycle and u_1, then $\det(\tilde{B}_H^{(1)}) = 0$.

Hence it implies that if $\det(\tilde{B}_H^{(1)}) \neq 0$ then $H = T \cup C_1 \cup ... \cup C_k$ where $u_1 \in T$ where T is a tree and $C_1 \cup ... \cup C_k$ are odd unicycles. Now if $H = T \cup C_1 \cup ... \cup C_k$ where $u_1 \in T$ where T is a tree and $C_1 \cup ... \cup C_k$ are odd unicycles, then $\tilde{B}_H^{(1)}$ is of the form

$$\tilde{B}_H^{(1)} = \left(\begin{array}{c|c|c|c} \tilde{B}_T & 0 & ... & 0 \\ \hline 0 & \tilde{B}_{C_1} & ... & 0 \\ \hline \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ \hline 0 & ... & 0 & \tilde{B}_{C_k} \end{array}\right).$$

Note that $\det(\tilde{B}_T) = \pm 1$ (by [3]) and by expanding the determinant of the non-oriented incidence matrix of a cycle, we can show that $\det(\tilde{B}_{C_i}) = \pm 2$ (see Appendix for the details), which implies that

$$\left(\det(\tilde{B}_H^{(1)})\right)^2 = 4^{\omega(H)-1},$$

where $\omega(H)$ is the number of components in H. Furthermore, by [5],

$$\det(Q) = \sum_{H \in C_0} 4^{\omega(H)}$$

and it follows that

$$\varepsilon_{QW} = \frac{\sum\limits_{H \in \mathcal{T}\mathcal{C}_o} 4^{\omega(H)-1}}{\sum\limits_{H \in C_0} 4^{\omega(H)}}$$

which completes the proof. □

3.6 Example

As an example to our result in Theorem 3.11, we consider the connected graphs with 4 vertices labeled by $\{u_1, u_2, u_3, u_4\}$. The setting is the same as in Theorem 3.11 and we choose the inflow $\boldsymbol{\alpha} = (1, 0)$ at the vertices u_1 and u_4, respectively. We classify these graphs into 10 classes based on the number of edges, bipartiteness and the configuration of u_1 and u_4 and the numbers of important factors state in Definition 3.10. Note that the comfortability for the non-bipartite case depends *only* on u_1. We conclude that every graph with 4 vertices belongs to exactly one of the following classes (see Fig 3.3):

$$\mathcal{G}_1 = \{K_4\},$$

$$\mathcal{G}_2 = \{K_4 - u_1 u_j : j = 2, 3, 4\},$$
$$\mathcal{G}_3 = \{K_4 - u_i u_j : i, j = 2, 3, 4\},$$
$$\mathcal{G}_4 = \{C_4 : u_1 \sim u_4\},$$
$$\mathcal{G}_5 = \{C_4 : u_1 \nsim u_4\},$$
$$\mathcal{G}_6 = \{G : G \text{ is constructed by joining } u_1 \text{ to exactly one vertex in the cycle } u_2, u_3, u_4\},$$
$$\mathcal{G}_7 = \{G : G \text{ is constructed by joining } u_i (i = 2, 3, 4) \text{ to exactly one vertex in the cycle } u_1, u_k, u_l (k, l \neq 1, i)\},$$
$$\mathcal{G}_8 = \{T : T \text{ is a tree with } \operatorname{dist}(u_1, u_4) = 1\},$$
$$\mathcal{G}_9 = \{T : T \text{ is a tree with } \operatorname{dist}(u_1, u_4) = 2\},$$
$$\mathcal{G}_{10} = \{T : T \text{ is a tree with } \operatorname{dist}(u_1, u_4) = 3\}.$$

Here $K_4 - u_i u_j$ is the graph obtained by removing the edge $u_i u_j$ from K_4. Now for $G_i \in \mathcal{G}_i (i = 1, ..., 10)$, we compute ε_{QW} as follows. When $G_0 = K_4$ for example, since K_4 is non-bipartite, we have

$$\varepsilon_{QW}(K_4) = \frac{\iota_2(K_4; u_1)}{\iota_1(K_4)}.$$

To compute $\iota_1(K_4)$, we need to find the number of odd unicyclic subgraphs which span K_4. The only such possible subgraph is a 3-cycle with an additional edge. It is clear that there are 4 ways to choose a 3-cycle and for a chosen 3-cycle, there are 3 ways to choose an edge which connects the remaining vertex to the cycle. Hence, altogether there are 12 such subgraphs, which are shown as $\mathcal{C}_o$ in figure 3.2. Observe that each subgraph has only one component and hence we have

$$\iota_1(K_4) = 48.$$

Now to compute $\iota_2(K_4; u_1)$, we have to find the spanning subgraphs which contains a tree with u_1 and the remaining are odd cycles, which are possibly empty. There are two types of such subgraphs, as shown as $\mathcal{TC}_o$ in figure 3.2 one being the spanning trees and the other being the cycle u_2, u_3, u_4 along with the single vertex u_1. In the first case the number of spanning trees is the tree number, or the complexity, of K_4, given by $4^{4-2} = 4^2$ (e.g., [3]) while in the second case there is only one such subgraph which has two components. So it follows that

$$\iota_2(K_4; u_1) = 20$$

and hence

$$\varepsilon_{QW}(K_4) = \frac{20}{48} = \frac{5}{12}.$$

Now consider $G_4 \in \mathcal{G}_4$. This graph is a 4-cycle with $u_1 \sim u_4$. This graph is bipartite and hence

$$\varepsilon_{QW}(G_4) = \frac{1}{4}\left(\frac{\chi_2(G_4; u_1, u_4)}{\chi_1(G_4)} + |E_0|\right).$$

Since $\chi_1(G_4)$ is the tree number of G_4 and by removing an edge from G_4 we can get a spanning tree, we have

$$\chi_1(G_4) = 4.$$

To compute $\chi_2(G_4; u_1, u_4)$, we have to find the number of forests with exactly two components, one containing u_1 and the other containing u_4. To find such a forest, the edge $\{u_1, u_4\}$ has to be removed, and other than that, one of the remaining edges has to be removed. So we have

$$\chi_2(G_4; u_1, u_4) = 3$$

and hence

$$\varepsilon_{QW}(G_4) = \frac{1}{4}(\frac{3}{4} + 4) = \frac{19}{16}.$$

Similarly, we compute the comfortability on the remaining classes of graphs and we tabulate these values as shown in Table 1.

$\mathcal{G}_i$	$\mathcal{G}_1$	$\mathcal{G}_2$	$\mathcal{G}_3$	$\mathcal{G}_4$	$\mathcal{G}_5$	$\mathcal{G}_6$	$\mathcal{G}_7$	$\mathcal{G}_8$	$\mathcal{G}_9$	$\mathcal{G}_{10}$
$\varepsilon_{QW}(\mathcal{G}_i)$	5/12	3/4	1/2	19/16	5/4	7/4	3/4	1	5/4	3/2
Scattering	R	R	R	T	T	R	R	T	T	T
Bipartiteness	-	-	-	○	○	-	-	○	○	○
$\|E\|$	6	5	5	4	4	4	4	3	3	3

Table 3.1: The comfortability of quantum walker to graphs with four vertices: The comfortability to each graph class is described by $\mathcal{E}_{QW}$. The symbols of "R" and "T" mean the perfect reflection and transmitting, respectively. The best graph with four vertices of the comfortability is the $\mathcal{G}_6$ and the worst graph is the complete graph.

Based on ε_{QW}, we have the following ordering of graphs:

$$G_6 \succ_{QW} G_{10} \succ_{QW} G_5, G_9 \succ_{QW} G_4 \succ_{QW} G_8 \succ_{QW} G_2, G_7 \succ_{QW} G_3 \succ_{QW} G_1.$$

Furthermore, we remark that for a tree T in general, with n vertices, the comfortability of the quantum walker is given by

$$\varepsilon_{QW}(T) = \frac{1}{4}\left(\mathrm{dist}(u_1, u_n) + (n-1)\right).$$

Finally we also consider the comparison between the comfortability for $z = 1$ and $z = -1$ cases. Any graph of four vertices is isomorphic to one of the graphs $\Gamma_1, \Gamma_2, \ldots, \Gamma_6$ given in Figure 3.4.

We set

$$\mathrm{Comf}(G) = \max_{u_1, u_n \in V(G)} \mathcal{E}_{QW}(G; \boldsymbol{\alpha}, u_1, u_n)$$

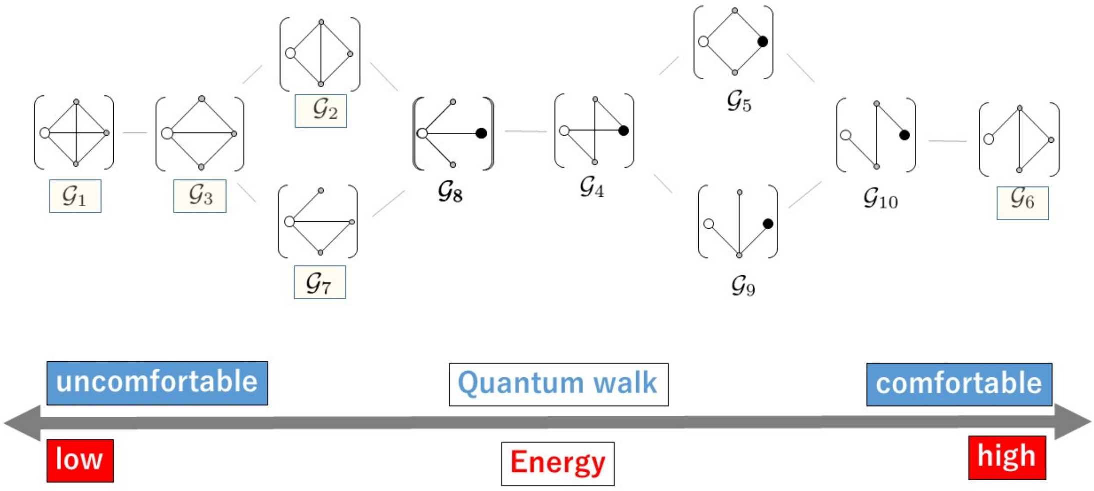

Figure 3.3: The Hasse diagram of comfortability of graphs: The most comfortable graph for this quantum walker is $\mathcal{G}_6$ which is a non-bipartite graph, while the most uncomfortable graph is $\mathcal{G}_1$ (the complete graph). Here the entrance vertex u_1 is indicated by the white vertex, and the exit vertex u_N is indicated by the black vertex for the bipartite case. Note that in the non-bipartite case, the comfortability for this quantum walker is independent of the position of the exit vertex (see Theorem 3.11).

	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6
$z=-1$	5/4	3/2	5/4	7/4	3/4	5/12
$z=1$	5/4	3/2	5/4	17/12	3/2	13/8

Table 3.2: $\mathrm{Comf}(\Gamma_j)$ for $z = \pm 1$

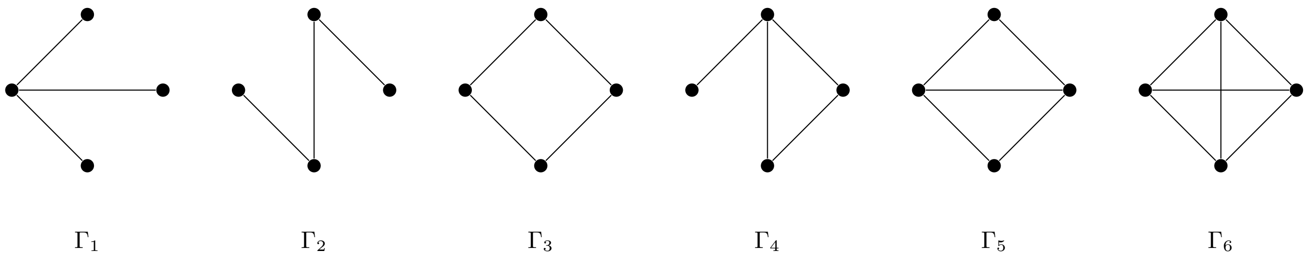

Figure 3.4: Non-isomorphic graphs Γ_j's for four vertices

for $\boldsymbol{\alpha} = (1, 0)$ at u_1 and u_n. Then we have the comfortabilities for each graph and $z = \pm 1$ as in Table 3.2. Thus we have, for $z = -1$,

$$\mathrm{Comf}(\Gamma_6) < \mathrm{Comf}(\Gamma_5) < \mathrm{Comf}(\Gamma_1) = \mathrm{Comf}(\Gamma_3) < \mathrm{Comf}(\Gamma_2) < \mathrm{Comf}(\Gamma_4),$$

and for $z = 1$,

$$\mathrm{Comf}(\Gamma_1) = \mathrm{Comf}(\Gamma_3) < \mathrm{Comf}(\Gamma_4) < \mathrm{Comf}(\Gamma_2) = \mathrm{Comf}(\Gamma_5) < \mathrm{Comf}(\Gamma_6).$$

Chapter 4

A quantum search on complete graphs

4.1 Setting

In this section, we introduce a quantum search algorithm using the tailed model. Note that, as we explained in the introduction, our goal is to utilize the properties obtained by the convergence in our model, we are particularly interested about the finding probability of a particular vertex in the long run. Now let us explain the setting and the notations in our study.

Let $G_0 = K_N$ be the complete graph with N number of vertices. We connect N tails $\{\mathbb{P}_j : j = 1, ..., N\}$ to every vertex of the graph, namely $\{u_1, ..., u_N\}$. We choose a vertex u_* as a marked vertex and we define the time evolution operator U as follows.

$$(U)_{a,b} = \begin{cases} -\left(\dfrac{2}{\deg(o(a))} - \delta_{a\bar{b}}\right) & \text{if } o(a) = t(b) = u_*, \\ \left(\dfrac{2}{\deg(o(a))} - \delta_{a\bar{b}}\right) & \text{if } o(a) = t(b) \neq u_*, \\ 0 & \text{otherwise.} \end{cases} \tag{4.1}$$

The state of the walker after time step t is $\Psi_t \in \mathbb{C}^{\tilde{A}}$ and can be computed by $\Psi_t = U\Psi_{t-1}$. The initial state $\Psi_0 \in \mathbb{C}^{\tilde{A}}$ is defined as follows.

$$\Psi_0(a) = \begin{cases} 1 & \text{if } a \in \tilde{A} \setminus A,\ \mathrm{dist}(t(a), K_N) < \mathrm{dist}(o(a), K_N) \\ 0, & \text{otherwise,} \end{cases} \quad (a \in \tilde{A}), \tag{4.2}$$

where $\mathrm{dist}(u, K_N)$ is the shortest distance between u and K_N. It is known from [14] that the following theorem holds.

Theorem 4.1. *There exists $\Psi_\infty \in \mathbb{C}^\infty$ such that, for any $a \in \tilde{A}$*

$$\lim_{t\to\infty} \Psi_t(a) = \Psi_\infty(a).$$

The relative probability of finding the vertex u_* at time t is given by

$$\tilde{\nu}_t(u_*) = \sum_{a\in A_0 : t(a)=u_*} |\psi_t(a)|^2.$$

Note that due to the initial state defined in equation 4.2, it acts as an external input to the graph, hence $\tilde{\nu}_t$ does not describe a probability. To normalize it, we set

$$\nu_t(u) := \frac{\tilde{\nu}_t(u)}{\sum_{v\in V(K_N)} \tilde{\nu}_t(v)}.$$

4.2 A search algorithm

It is noted that in our setup, when the operator U is applied $t_{run} = \lfloor \pi\sqrt{N} \rfloor$ times, the finding probability of u_* is higher, where we have a similar phenomena as the usual quantum search algorithms; that is we have $t_{run} = O(\sqrt{N})$. The difference in our model is that the state of the walker converges and hence the finding probability. Therefore we are particularly interested in the finding probability in the long run. First let us set up some basic results we use in the main theorems in this section.

4.2.1 An invariant subspace

It can be noted by the symmetricity of the walk, that there are 3 types of arcs which are partitioned into the disjoint sets A_+, A_-, A_* as follows.

$$\begin{aligned} A_+ &= \{a \in A_0 \ : \ t(a) = u_*\}, \\ A_- &= \{a \in A_0 \ : \ o(a) = u_*\}, \\ A_* &= \{a \in A_0 \ : \ t(a),\ o(a) \neq u_*\}. \end{aligned}$$

Also from the symmetricity of the time evolution, it is easy to notice that the value $\Psi_t(a)$ is invariant of the subsets A_+, A_- and A_*. Thus setting $a_t = \Psi_t(a)$ $(a \in A_+)$, $b_t = \Psi_t(a)$ $(a \in A_-)$ and $c_t = \Psi_t(a)$ $(a \in A_*)$, from the dynamics we have in (4.1), we obtain

$$\begin{bmatrix} a_{t+1} \\ b_{t+1} \\ c_{t+1} \end{bmatrix} = \begin{bmatrix} 0 & -1 + \dfrac{2}{N} & 2 - \dfrac{4}{N} \\ -1 + \dfrac{2}{N} & 0 & 0 \\ 0 & \dfrac{2}{N} & 1 - \dfrac{4}{N} \end{bmatrix} \begin{bmatrix} a_t \\ b_t \\ c_t \end{bmatrix} + \frac{2}{N} \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix}.$$

We can project this walk on to a path by normalizing these probability amplitudes a_t, b_t and c_t. To obtain this projected walk, we normalize these as follows,

$$\alpha_t := \begin{bmatrix} \sqrt{N-1} & 0 & 0 \\ 0 & \sqrt{N-1} & 0 \\ 0 & 0 & \sqrt{(N-1)(N-2)} \end{bmatrix} \begin{bmatrix} a_t \\ b_t \\ c_t \end{bmatrix}.$$

Thus we obtain the following master equation:

$$\alpha_{t+1} = T(\epsilon)\alpha_t + b_\epsilon, \ \alpha_0 = 0. \tag{4.3}$$

Here

$$T(\epsilon) = \begin{bmatrix} 0 & -1 + \epsilon^2 & \sqrt{2\epsilon^2(1-\epsilon^2)} \\ -1 + \epsilon^2 & 0 & 0 \\ 0 & \sqrt{2\epsilon^2(1-\epsilon^2)} & 1 - 2\epsilon^2 \end{bmatrix}$$

and

$$b_\epsilon = \left[\epsilon\sqrt{2-\epsilon^2},\ -\epsilon\sqrt{2-\epsilon^2},\ \sqrt{4 - 6\epsilon^2 + 2\epsilon^4}\right]^\top,$$

where $\epsilon = \sqrt{\dfrac{2}{N}}$.

Remark that the relative probability of the marked vertex can be computed by $\nu_t(u_*) = ||\alpha_t(1)||^2$. Now let us consider the asymptotics for large N, which is equivalent to considering (4.3) for small perturbation ϵ. Also by solving the recursion in equation 4.3, we obtain the following.

$$\alpha_t = \left(I + T(\epsilon) + T^2(\epsilon) + \cdots + T^{t-1}(\epsilon)\right) b_\epsilon.$$

And we use perturbation theory on $T(\epsilon)$ to approximate α_t.

4.2.2 Kato's perturbation theory on $T(\epsilon)$

Observe that $T(\epsilon)$ can be expanded using the Maclaurin series as follows.

$$T(\epsilon) = T_0 + \epsilon T_1 + \epsilon^2 T_2 + \cdots ,$$

where

$$T_0 = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 2 \end{bmatrix}, \tag{4.4}$$

which is symmetric and hence diagonalizable. Note that the spectrum of T_0 is $\mathrm{Spec}(T_0) = \{-1, 1, 1\}$, hence we can use the degenrate perturbation to approximate the eigenvalues and eigenvectors of T_0. Moreover, we have

$$T_1 = \begin{bmatrix} 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{bmatrix}$$

and

$$T_2 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -2 \end{bmatrix}.$$

Now let us explain the expansions of the eigenvalues and the projection operators on to the corresponding eigenspaces. Since the spectrum of T_0 is $\mathrm{Spec}(T_0) = \{-1, 1, 1\}$, we can use the degenerate perturbation in [15]. Denote the eigenvalue of $T(\epsilon)$ which corresponds to -1 by $\lambda_{-1}(\epsilon)$ and the two eigenvalues corresponding to 1 by $\lambda_{1,\pm}(\epsilon)$ and the expansions are given as follows.

$$\lambda_{-1}(\epsilon) = -1 + \epsilon\lambda_{-1}^{(1)} + \epsilon^2\lambda_{-1}^{(2)} + O(\epsilon^3) \tag{4.5}$$

$$\lambda_{1,\pm}(\epsilon) = 1 + \epsilon\lambda_{1,\pm}^{(1)} + o(\epsilon) + \cdots \tag{4.6}$$

Since -1 is a simple eigenvalue of T_0, the coefficients $\lambda_{-1}^{(1)}$ and $\lambda_{-1}^{(2)}$ are given as follows.

$$\lambda_{-1}^{(1)} = \mathrm{tr}(T_1 P_{-1}), \tag{4.7}$$

$$\lambda_{-1}^{(2)} = \mathrm{tr}(T_2 P_{-1} - T_1 S_{-1} T_1 P_{-1}), \tag{4.8}$$

where P_λ is the eigenprojection corresponding to the eigenvalue λ and S_λ is the reduced resolvent at λ ($\lambda \in \mathrm{Spec}(T)$) which can be computed using

$$P_{-1} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{3} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

and

$$\begin{aligned} S_{-1} &= -\lim_{\xi \to -1} \sum_{\lambda \in \mathrm{Spec}(T) \setminus \{-1\}} (\xi - \lambda)^{-1} P_\lambda = \frac{1}{2}(I - P_{-1}) \\ &= \frac{1}{2} \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}. \end{aligned}$$

Thus we have

$$\lambda_{-1}^{(1)} = 0$$

and

$$\lambda_{-1}^{(2)} = \frac{1}{2}.$$

Hence, we obtain

$$\lambda_{-1}(\epsilon) = -1 + \frac{1}{2}\epsilon^2 + O(\epsilon^3). \tag{4.9}$$

Since 1 is a semi-simple eigenvalue of T_0, to compute $\lambda_{1,\pm}(\epsilon)$, we use the reduction process given in [15]. Consider

$$\tilde{T}(\epsilon) := \frac{1}{\epsilon}(T(\epsilon) - 1)P_1(\epsilon).$$

Here $P_1(\epsilon)$ is the total projection for the +1-group. The new matrix $\tilde{T}(\epsilon)$ can be expanded by

$$\tilde{T}(\epsilon) = \tilde{T}_0 + \epsilon\tilde{T}_1 + \cdots$$

because +1 is semi-simple eigenvalue of T. Here $\tilde{T}_0$ is computed using the results given in [15]:

$$\begin{aligned}\tilde{T}_0 &= P_1 T_1 P_1 \\ &= \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 1 \\ 1 & -1 & 0 \end{bmatrix}.\end{aligned}$$

Using this expression for $\tilde{T}_0$ the coefficient $\lambda_{1,\pm}^{(1)}$ can be obtained from the spectrum of $\tilde{T}_0$ as follows:

$$\lambda_{1,\pm}^{(1)} \in \operatorname{Spec}\left(\tilde{T}_0|_{(P_1)}\right) = \{\pm i\},$$

and the corresponding eigenvectors are given by

$$v_{1,\pm i} = \frac{1}{2}\,[\mp i,\ \pm i,\ \sqrt{2}]^\top.$$

Since $\tilde{T}_0$ is a skew-Hermitian matrix, the eigenprojections of $\pm i$ can be directly computed by its normalized eigenvectors $v_{1,\pm i}$ as

$$P_{1,\pm} := v_{1,\pm} v_{1,\pm i}^*$$

and it can be checked that

$$P_1 = v_{1,+i}v_{1,+i}^* + v_{1,-i}v_{1,-i}^*.$$

Moreover, since the eigenvalues $\pm i$ are simple, the term $o(\epsilon)$ of the expansion of $\lambda_{1,\pm}(\epsilon)$ can be expressed by

$$o(\epsilon) = \epsilon^2\lambda_{1,\pm}^{(2)} + O(\epsilon^3)$$

and the coefficient $\lambda_{1,\pm}^{(2)}$ can be obtained by using the formula of the weighed mean of the perturbed eigenvalues again; that is,

$$\lambda_{1,\pm}^{(2)} = \operatorname{tr}\left(\tilde{T}_0 P_{1,\pm}\right) = -\frac{5}{4}.$$

And finally, we obtain the rest of the eigenvalues of $T(\epsilon)$ as follows.

$$\lambda_{1,\pm}(\epsilon) = 1 \pm i\epsilon - \frac{5}{4}\epsilon^2 + O(\epsilon^3). \tag{4.10}$$

Now with the approximations of the eigenvalues, we can write the spectral decomposition of $T(\epsilon)$ which is given by

$$T(\epsilon) = \lambda_{-1}(\epsilon)P_1(\epsilon) + \lambda_{1,+}(\epsilon)P_{1,+}(\epsilon) + \lambda_{1,-}(\epsilon)P_{1,-}(\epsilon),$$

where $P_j(\epsilon)$ is the eigenprojection onto the each perturbed eigenvalues and can be expanded by

$$P_j(\epsilon) = P_j + O(\epsilon).$$

This implies

$$\alpha_t = \left(\frac{1-\lambda_{-1}^t(\epsilon)}{1-\lambda_{-1}(\epsilon)} P_{-1}(\epsilon) + \frac{1-\lambda_{1,+}^t(\epsilon)}{1-\lambda_{1,+}(\epsilon)} P_{1,+}(\epsilon) + \frac{1-\lambda_{1,-}^t(\epsilon)}{1-\lambda_{1,-}(\epsilon)} P_{1,-}(\epsilon) \right) b_\epsilon. \tag{4.11}$$

Inserting the expansions of $\lambda_{-1}(\epsilon)$, $\lambda_{1,\pm}(\epsilon)$ in (4.9), (4.10) into (4.11), we have the following expression for α_t:

$$\begin{aligned} \alpha_t &= \frac{1}{2} \left\{ 1 - (-1)^t e^{-\frac{\epsilon^2 t}{2}(1+O(\epsilon))} \right\} e^{\frac{\epsilon^2}{4}(1+O(\epsilon))} b_\epsilon^{(-1)} \\ &+ \frac{i}{\epsilon} \left\{ 1 - e^{i\epsilon t} e^{-\frac{5}{4}\epsilon^2 t(1+O(\epsilon))} \right\} e^{\frac{5}{4} i\epsilon(1+O(\epsilon))} b_\epsilon^{(1,+)} \\ &- \frac{i}{\epsilon} \left\{ 1 - e^{-i\epsilon t} e^{-\frac{5}{4}\epsilon^2 t(1+O(\epsilon))} \right\} e^{-\frac{5}{4} i\epsilon(1+O(\epsilon))} b_\epsilon^{(1,-)}. \end{aligned} \tag{4.12}$$

Here $b_\epsilon^{(j)} := P_j(\epsilon) b_\epsilon$. We notice that $P_{-1} b_0 = 0$, which implies that there exists b' such that $b_\epsilon^{(-1)} = \epsilon(b' + O(\epsilon))$.

4.2.3 Theorems on the quantum search driven by the tailed model

Now let us give the main theorems in this section. Comparing to the usual quantum walk search algorithms, we have a similar theorem as follows, which gives a run-time of the order $O(\sqrt{N})$ to get a maximum finding probabilty of u_*.

Theorem 4.2. (Pulsation) *Until the time step $O(N)$, the finding probability of the marked vertex is estimated by*

$$\nu_t(u_*) \sim \frac{1}{2} \frac{(\ 1 - c_t \cos[t\sqrt{2/N}]\ )^2}{1 + c_t^2},$$

where $c_t = e^{-(5/2)\cdot(t/N)}$ for large size N. In particular, at the time step $t \sim \pi\sqrt{N/2}$, the finding probability of the marked vertex is

$$\nu_t(u_*) \sim \frac{1}{2} \frac{(\ 1 + e^{-\frac{5\pi}{2\sqrt{2N}}}\ )^2}{1 + e^{-\frac{5\pi}{\sqrt{2N}}}} > \frac{1}{2}.$$

Proof. Since $b_\epsilon^{(-1)} \in O(\epsilon)$, if $t \ll 1/\epsilon^2$, the second and third terms in (4.12) are main terms; that is,

$$\alpha_t \sim \frac{i}{\epsilon}(1 - e^{i\epsilon t} e^{-\frac{5}{4}\epsilon t^2}) b_\epsilon^{(1,+)} - \frac{i}{\epsilon}(1 - e^{-i\epsilon t} e^{-\frac{5}{4}\epsilon t^2}) b_\epsilon^{(1,-)}$$

for sufficiently small ϵ. Note that

$$\begin{aligned} b_\epsilon^{(1,+)} &= P_{1,+} b_\epsilon = \langle v_{1,i}, b_0 \rangle v_{1,i} + O(\epsilon) \\ &= [-i/\sqrt{2}, i/\sqrt{2}, 1]^\top + O(\epsilon). \\ b_\epsilon^{(1,-)} &= P_{1,-} b_\epsilon = \langle v_{1,-i}, b_0 \rangle v_{1,-i} + O(\epsilon) \\ &= [i/\sqrt{2}, -i/\sqrt{2}, 1]^\top + O(\epsilon). \end{aligned}$$

Therefore until $t \in O(1/\epsilon)$, we have

$$\alpha_t \sim \frac{i}{\epsilon} \left[-\sqrt{2}(1 - c_t \cos \epsilon t),\ \sqrt{2}(1 + c_t \cos \epsilon t),\ 2 \sin \epsilon t \right]^\top,$$

where $c_t = e^{-(5/4)\epsilon^2 t}$. Then the normalized constant of the relative probability can be computed by $4(1 + c_t^2)$. Then we have

$$\nu_t(u_*) \sim \frac{2(1 - c_t \cos \epsilon t)^2}{4(1 + c_t^2)},$$

for $t \in O(1/\epsilon)$. In particular, if $t = \pi/\epsilon$, then the finding probability at the marked vertex takes the local maximal value

$$\nu_t(u_*) = \frac{1}{2}\frac{(1+e^{-5\pi/(2\sqrt{2N})})^2}{1+e^{-5\pi/\sqrt{2N}}} > 1/2.$$

□

This theorem implies that until the time step $O(N)$, this walk has the oscillation with the periodicity $\pi\sqrt{2N}$. Thus the locally maximal value of the time sequence of $\{\mu_t(u_*)\}_{t>0}$ can be observed around $O(\sqrt{N})$ and its probability is higher than 1/2.

Next we answer the natural question arised in our model, *What is the behaviour of the finding probability in the long run?*

Definition 4.3. (The limit distribution) *The normalized finding probabilty on $V(K_N)$ is defined by*

$$\mu_N(u) = \lim_{t\to\infty} \nu_t(u)$$

for any $u \in V(K_N)$.

Theorem 4.4. (The finding probability of the marked vertex at the fixed point)
Let μ be the limit distribution of the finding probability defined as the above. Then we have

$$\lim_{N\to\infty} \mu_N(u_*) = \frac{1}{2}.$$

Proof. Taking $t \to \infty$ in (4.11) and inserting the expansions of $\lambda_{-1}(\epsilon)$ and $\lambda_{1,\pm}(\epsilon)$ in (4.9) and (4.10), we have

$$\begin{aligned}\alpha_\infty &:= \lim_{t\to\infty} \alpha_t \\ &= \frac{1}{2}e^{\epsilon^2(1+O(\epsilon))/4}P_{-1}(\epsilon)b_\epsilon + \frac{i}{\epsilon}e^{5i\epsilon(1+O(\epsilon))/4}P_{1,+}(\epsilon)b_\epsilon - \frac{i}{\epsilon}e^{-5i\epsilon(1+O(\epsilon))/4}P_{1,-}(\epsilon)b_\epsilon.\end{aligned}$$

Then

$$\begin{aligned}\lim_{\epsilon\to 0}\epsilon\alpha_\infty &= \lim_{\epsilon\to 0}(ie^{5i\epsilon/4}P_{1,+}(\epsilon)b_\epsilon - ie^{-5i\epsilon/4}P_{1,-}(\epsilon)b_\epsilon) \\ &= \lim_{\epsilon\to 0} 2\mathrm{Re}\left(ie^{5i\epsilon/4}P_{1,+}b_\epsilon\right) \\ &= -2\mathrm{Im}(P_{1,+}b_0) \\ &= \frac{-1}{\sqrt{2}}\begin{bmatrix}-i\\ i\\ 0\end{bmatrix}.\end{aligned}$$

Thus the finding probability at the target vertex u_* is 1/2 because the relative probability is given by $|\alpha_\infty(1)|^2$. □

This theorem implies that we can find the marked vertex in the stable state with probability 1/2 while the traditional quantum search algorithm has the oscillation. Since the traditional quantum search algorithm takes $O(\sqrt{N})$ if we measure the system at an appropriate time, now the next interest may be that *how long does it take to converge?* To answer the question, let us introduce the finite time which we regard as convergence.

Definition 4.5. (ℓ^2-mixing time of quantum walk) *Let Ψ_t be the t-th iteration of the quantum walk and Ψ_∞ be its stationary state. For $\theta > 0$, we set $t(\theta)$ by*

$$t(\theta) := \min\{s > 0 \ : \ {}^\forall t > s,\ ||\Psi_\infty - \Psi_t||_{K_N} < e^{-\theta}\},$$

where for $f \in \mathbb{C}^{\tilde{A}}$, the norm $||f||_{K_N}$ is the ℓ^2-norm with respect the internal graph; that is,

$$||f||^2_{K_N} := \sum_{a\in A:\ t(a)\in V(K_N)} |f(a)|^2.$$

Theorem 4.6. (The ℓ^2-mixing time) *Let $t(\theta)$ be the ℓ^2-valued mixing time defined as the above. Then we have*

$$t(\theta) \in \Theta(N \log N)$$

for any fixed $\theta > 0$.

Proof. By (4.12), we have

$$||\alpha_\infty - \alpha_t|| = \frac{e^{-\frac{\epsilon^2 t}{2}(1+o(1))}}{\epsilon} \left|\left|\frac{\epsilon^2}{2}(-1)^t(b' + o(1)) + ie^{-\frac{3}{4}\epsilon^2 t}(b_0^{(1,+)} + o(1)) - ie^{-\frac{3}{4}\epsilon^2 t}(b_0^{(1,-)} + o(1))\right|\right|. \tag{4.13}$$

There is a conflict between ϵ^2 and $e^{-3\epsilon^2 t/4}$ in the RHS. Note that $\epsilon^2 \ll e^{-3\epsilon^2 t/4}$ if and only if $t < 8|\log \epsilon|/(3\epsilon^2)$. Let us see the lower bound of t such that $||\alpha_\infty - \alpha_t|| < e^{-\theta}$ if $t < 8|\log \epsilon|/(3\epsilon^2)$. By (4.13), there exists $m > 0$ such that

$$||\alpha_\infty - \alpha_t|| = (m + o(1))\frac{e^{-\frac{5\epsilon^2 t}{4}(1+o(1))}}{\epsilon}. \tag{4.14}$$

Then solving

$$(m + o(1))\frac{e^{-\frac{5\epsilon^2 t}{4}(1+o(1))}}{\epsilon} < e^{-\theta},$$

we obtain the lower bound of t by

$$t > (\theta + \log(m + o(1)) + |\log \epsilon|)\frac{4}{5\epsilon^2(1 + o(1))}.$$

Thus the lower bound of such a t must belong to at least $\Theta(|\log \epsilon|/\epsilon^2)$. On the other hand, if $t \geq 8|\log \epsilon|/(3\epsilon)^2$, then (4.13) is rewritten by

$$||\alpha_\infty - \alpha_t|| = (m' + o(1))\epsilon e^{-\frac{\epsilon^2 t}{2}(1+o(1))}, \tag{4.15}$$

which implies

$$t > (\theta + \log(m' + o(1)) - |\log \epsilon|)\frac{2}{\epsilon^2(1 + o(1))}.$$

Since $t > 8|\log \epsilon|/(3\epsilon)^2$, this inequality is satisfied for any fixed θ if ϵ is sufficiently small. Therefore we can conclude that $t(\theta) \in \Theta(|\log \epsilon|/\epsilon^2) = \Theta(N \log N)$. □

Remark. *We remark that theorems 4.2 and 4.6 both give finding probabilities in their unique ways, where the former one gives a quantum speed-up and the latter one shows a stability. In other words, the former one appears to be a finding probability which is in usual quantum walk based search algorithms and the latter one occurs because of the converging property of our model which shows a speed down and takes more time than classical search algorithms, but has advantage in measuring as the finding probability is stable.*

Chapter 5

Conclusion

Discrete time quantum walks is the quantum analogy of random walks, which is determined by a set of states in the Hilbert space spanned by the set of arcs of the underlying graph, and a unitary operator which describes the dynamics that changes the state of the walker at each time step. In general, it is not necessary that the state of the walker converges, because the time evolution operator is unitary, and hence the eigenvalues lie on the unit circle. We introduce the tailed model which guarantees the convergence of the state in the long run. The state which the state of the walker converges to is called the stationary state. This property is new to the tailed model and we are interested in utilizing it and study the use of this stationary state in various situations.

First we study the Szegedy dynamics in the tailed model. We show that in the long run, the scattering matrix of the walker becomes the Szegedy matrix. Moreover, we define an electric current function in terms of the stationary state and we show that this current function satisfies the Kirchhoff's current and voltage laws.

Next we study a Grover-like dynamics in the tailed model, which is equivalent to a special case of a previously known model. In this study we find the scattering matrix and show that the scattering matrix gives a characterization of bipartite graphs. Based on this characterization, if the underlying graph is bipartite or non-bipartite, we derive a current function and a pseudo-current function respectively, which satisfy Kirchhoff laws and a type of pseudo-Kirchhoff laws respectively. Moreover, we formulate the electric network equations using the Laplacian and signless-Laplacian matrices of the underlying graph respectively. Furthermore, we introduce the notion of the comfortability of the underlying graph, a quantum analogy of the energy of the electric circuit and using the properties of the Laplacian and the signless-Laplacian matrices, we obtain the comfortability of the underlying graphs in terms of the combinatorial properties of the graph. If the underlying graph is bipartite, we show that the comfortability can be computed in terms of the tree number and the number of spanning forests of the graph and if the underlying graph is non-bipartite, we show that it can be computed in terms of the odd unicyclic subgraphs.

Finally, we study a quantum search algorithm on the complete graph K_N, which arises from the tailed model. Unlike the usual quantum search algorithm in the literature, since the state of the walker converges in our model, we have two types of finding probabilities for a given marked vertex. The first type of the finding probability is a maximum finding probability obtained at a time step of order $O(\sqrt{N})$, which is a similar result to the usual quantum search algorithms. The second type of the finding probability is the probability obtained at the stationary state, or the limiting probability in the long run. This type of finding probability arises due to the convergence property in our model which is not achieved in the usual quantum search algorithms. We show that this limiting probability is arbitrary close to $\frac{1}{2}$ when the order of the run-time of the algorithms is as large as $O(N \log N)$.

Appendix

Let C_i be an odd unicyclic graph and let $\tilde{B}_{C_i}$ be the non-oriented incident matrix of C_i. Let us prove that $\det(\tilde{B}_{C_i}) = \pm 2$. Since an odd unicyclic graph is obtained by connecting trees to an odd cycle (say C'), If we expand $\det(\tilde{B}_{C_i})$ along the row corresponding to a leaf of a tree connected to C', it reduces to a similar determinant. By expanding recursively along the rows corresponding to the leaves of the graph, we obtain

$$\det(\tilde{B}_{C_i}) = \pm\det(B_{C'}).$$

Now it is enough to show that $\det(B_{C'}) = 2$. Observe that we have

$$\det(B_{C'}) = \det\begin{pmatrix} 1 & 0 & ... & 0 & 1 \\ 1 & 1 & 0 & ... & 0 \\ . & . & & & \\ . & & . & & \\ . & & & . & \\ 0 & ... & 0 & 1 & 1 \end{pmatrix}.$$

Expanding the determinant in the right hand side along the first row, since there are odd number of rows and columns, we get

$$\det(B_{C'}) = \det\begin{pmatrix} 1 & 0 & ... & 0 & 0 \\ 1 & 1 & 0 & ... & 0 \\ . & . & & & \\ . & & . & & \\ . & & & . & \\ 0 & ... & 0 & 1 & 1 \end{pmatrix} + \det\begin{pmatrix} 1 & 1 & ... & 0 & 0 \\ 0 & 1 & 1 & ... & 0 \\ . & . & & & \\ . & & . & & \\ . & & & . & \\ 0 & ... & 0 & 0 & 1 \end{pmatrix}.$$

Now to compute the two determinants in the right hand side, we expand the first determinant recursively along the rows and the second along the columns and we obtain that these two determinants are equal to 1. Hence we conclude that

$$\det(\tilde{B}_{C_i}) = \pm 2.$$

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Bibliography

[1] Ambainis, A. (2003) Quantum walks and their algorithmic applications. *Int. J. Quantum Inf., 1 (04)*, 507-518.

[2] Balabanian, N., Bickart, T.A. (1969) Electrical Network Theory. John Wiley Sons, Inc.

[3] Biggs, N. (1993) Algebraic Graph Theory (2nd ed.). Cambridge University Press.

[4] Bollobás, B. (2013) Modern Graph Theory. Springer.

[5] Cvetkovic, D.M., Rowlinson, P. and Simic, S. (2007) Signless Laplacians of finite graphs. *Linear Algebra Appl. , 423(1),* 155-171.

[6] Cvetkovic, D.M., Rowlinson, P. and Simic, S. (2010) An introduction to the theory of graph spectra. Cambridge: Cambridge University Press.

[7] Feldman, E. and Hillery, M. (2005) Quantum walks on graphs and quantum scattering theory. *Contemp. Math. 381*, 71.

[8] Feldman, E. and Hillery, M. (2007) Modifying quantum walks: a scattering theory approach. *J. Phys. A: Math. Theor. 40*, 11343.

[9] Chris Godsil, Hanmeng Zhan, Discrete-Time Quantum Walks and Graph Structures, Journal of Combinatorial Theory, Series A 167 (2019) pp.181-212.

[10] Grover, L.K. (1997) Quantum mechanics helps in searching for a needle in a haystack. *Phys. Rev. Lett., 79(2)*, 325.

[11] Higuchi, Yu., Konno, N., Sato, I. and Segawa, E. (2014) Spectral and asymptotic properties of Grover walks on crystal lattices. *J. Funct. Anal. 267.,* 4197–4235.

[12] Higuchi, Yu., Sabri, M. and Segawa, E. (2020) Electric Circuit Induced by Quantum Walk. *J. Stat. Phys., 181,* 603-617.

[13] Higuchi, Yu. and Segawa, E. (2018) Quantum walks induced by Dirichlet random walks on infinite trees, *J. Phys. A: Math. Theor., 51,* 075303.

[14] Higuchi, Yu. and Segawa, E. (2019) A dynamical system induced by quantum walk. *J. Phys. A: Math. Theor., 52,* 395202.

[15] Kato, T. (2012). A short introduction to perturbation theory for linear operators. Springer Science Business Media.

[16] Konno, N. (2008) Quantum Walks, In: Quantum Potential Theory pp.309-452, Springer.

[17] Norio Konno, Masato Takei (2015) The non-uniform stationary measure for discrete-time quantum walks in one dimension. Quantum Inf. Comput. 15(11,12) pp.1060-1075.

[18] Manouchehri, K. and Wang, J. (2014) Physical Implementation of Quantum Walks. Springer.

[19] Jan Mareš, Jaroslav Novotný, Igor Jex, Percolated quantum walks with a general shift operator: From trapping to transport, Phys.Rev.A.99 (2019) 042129.

[20] Matsue, K., Matsuoka, L., Ogurisu, O., Segawa, E. (2019). Resonant-tunneling in discrete-time quantum walk. *Quantum Studies: Mathematics and Foundations, 6(1)*, 35-44.

[21] Portugal, R. (2018) Quantum Walks and Search Algorithms (2nd ed.). Springer.

[22] Seshu, S. and Reed, M. B. (1961) Linear Graphs and Electric Networks. Addison-Wesley Publishing Company, Inc.

[23] Shenvi, N., Kempe, J., and Whaley, K. B. (2003) Quantum random-walk search algorithm. *Phys. Rev. A, 67(5)*, 052307.

[24] Tanaka, H., Sabri, M., Portugal, R. (2022). Spatial search on Johnson graphs by discrete-time quantum walk. *Journal of Physics A: Mathematical and Theoretical.*

[25] Venegas-Andraca, S. E. (2008). Quantum walks for computer scientists. *Synthesis Lectures on Quantum Computing, 1(1).*