CHUNG-YAU INVARIANTS AND RANDOM WALK ON GRAPHS

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The Chung-Yau graph invariants were originated from Chung-Yau's work on discrete Green's function. They are useful to derive explicit formulas and estimates for hitting times of random walks on discrete graphs. In this thesis, we study properties of Chung-Yau invariants and apply them to study some questions:

(1) The relationship of Chung-Yau invariants to classical graph invariants;

(2) The change of hitting times under natural graph operations;

(3) Properties of graphs with symmetric hitting times;

(4) Random walks on weighted graphs with different weight schemes.

Keywords: random walk, hitting time, spanning tree, Chung-Yau invariants, Kemeny's constants, reversible graph.

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PREFACE

Pursuing this Ph.D degree over the past several years has been a joy and frustrating experience for me and I would like to deeply thank a great number of individuals who have made this special memory so treasurable.

First and foremost, I would like to give my sincere thanks to my advisors Professor Hao Xu and Professor Piotr Hajlasz. Without Professor Xu and Professor Hajlasz's constant support and encouragement, I would definitely not be able to made it so far.

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1.0 INTRODUCTION

A random walk on a graph is a process that a walker moves from vertices to vertices along edges such that at each step it moves to a neighboring vertex with equal probability. Random walks on graphs have been studied extensively in the literature, through various methods from a wide variety of subjects such as probability, spectral geometry and electric network. Besides being an important subject in mathematics, it has founded many applications in physics, chemistry, computer science, finance and biology.

Particularly, interesting parameters of random walks include the hitting time, commute time and cover time. The hitting time of a graph is defined to be the expected number of steps to go from one vertex to the other. The cover time is the expected number of steps to visit all vertices. By definition, the cover time is closely related to hitting time. For most special graphs such as path, cycle and complete graphs, their hitting or cover times are known. For general graph, we have classical formulas of hitting times expressed in terms of graph spectra or effective resistance. On the other hand, in the last fifty years, people have developed techniques to estimate the upper and lower bounds of hitting and cover times, to obtain optimal bounds and extremal graphs.

In this thesis, we focus on studying the hitting times for random walks on graphs. The main new contributions are contained in Chapter 4 to Chapter 6. In particular, Chapter 4 is based on the paper [20] and Chapter 5 is based on the paper [21].

Chapter 2 serves as an introduction to random walk on graphs. We first introduce fundamental materials on graph spectra and electric networks. Then we compute the hitting and cover times for 3 kinds of graphs: complete graph, path and cycle. In each case, we present several different methods (graph spectra, electric network, first step analysis, transition matrix technique) in computing the hitting time, to better give a comprehensive view of the difficulties and advantages of these approaches. We don't know any single textbook or paper that put together all these methods of calculating hitting times.

In Chapter 3, we introduce the Chung-Yau invariants for vertex-weighted graphs. They consist of R and Z-invariants arising from Chung-Yau's work on discrete Green's functions and random walks. We will discuss their basic properties and applications in the computation of discrete Green's functions and hitting times. This chapter was largely borrowed from [24, 25], but we tried to give alternative proofs to the main theorems and improved some results along the way.

In [25], building on the Chung-Yau invariants, an explicit formula of hitting times in terms of spanning trees (cf. Theorem 3.3.4) was proved. This is the starting point for most works in Chapters 4 to 6. It is not only an exact formula of hitting times but also can be used to recover almost all known identities and estimates of hitting times or even produce new ones involving only standard graph theoretic techniques. This approach completely avoids ingenious probabilistic arguments or knowledge about electric networks.

In Chapter 4, we apply the above mentioned formula to study the relationship of hitting times under graph operations. Let G be a connected graph. Two kinds of graph operations on G are considered. One is the graph $S_k(G)$ obtained by inserting k new vertices of degree 2 to each edge of G. The other is the graph $Q_k(G)$ obtained by adding a path of length k between any two adjacent vertices of G. We prove explicit formulas expressing hitting times of $S_k(G)$ (res. $Q_k(G)$) in terms of those of G. They generalized the previous works [5, 12] of other scholars for $k \leq 2$ with quite different methods.

Denoted by $S_k(G)$ the graph obtained from G by inserting k new vertices of degree 2 to each edge of G. Denote $V(S_k(G)) = V \cup V'$, where V is the set of original vertices in G, and V' is the set of newly inserted vertices.

If $i \in V'$ is inserted on the edge $st \in E(G)$, we will denote $\Gamma(i) = (s, t)$ and also regard i an integer $1 \leq i \leq k$ with $s = 0$ and $t = k + 1$. In fact, for $i \in V$ incident to an edge $st \in E(G)$, we also denote $\Gamma(i) = (s, t)$, we may regard $i = 0$ if $i = s$ and $i = k + 1$ if $i = t$.

Theorem 4.1.6 gives relations of hitting times on $S_k(G)$ to that of G.

Theorem 1.0.1. *If $i \in V \cup V'$, $j \in V \cup V'$, $\Gamma(i) = (s,t)$, $\Gamma(j) = (p,q)$, then*

$$\begin{aligned} H_{S_k(G)}(i,j) =&(k+1-i)(k+1-j)H_G(s,p) + (k+1-i)jH_G(s,q) \\ &+ i(k+1-j)H_G(t,p) + ijH_G(t,q) + i(k+1-i) - j(k+1-j) \\ &+ j(k+1-j)(2m - H_G(p,q) - H_G(q,p)) - \varepsilon(k,i,j). \end{aligned}$$

Here $\varepsilon(k,i,j)$ is given by

$$\varepsilon(k,i,j) = \begin{cases} 0, & \text{if } i,j \text{ are on different edges of } G; \\ 2mi(k+1-j), & \text{if } i,j \text{ are on the same edge of } G \text{ and } i \le j; \\ 2mj(k+1-i), & \text{if } i,j \text{ are on the same edge of } G \text{ and } i \ge j. \end{cases}$$

In Chapter 5, we establish identities of discrete Green's function and Kemeny's constant in terms of Chung-Yau invariants. Then we apply Chung-Yau invariants to study symmetric graphs, i.e., graphs with symmetric hitting times. A question of Geogarkopoulos asks that whether a reversible graph is walk-regular. We prove a partial result in this direction: If a regular graph G is reversible and not far from walk-regular, then G is walk-regular. Finally we prove a series of formulas showing the change of hitting times when an edge is added or removed from a graph.

In Proposition 5.1.4, we proved a formula of Kemeny's constant (see (2.7)) in terms of Chung-Yau invariants Z (see Definition 3.1.1).

Proposition 1.0.2. *Let G be a connected graph. Then*

$$K(G) = \frac{1}{\mathrm{vol}(G)^2\tau(G)} \sum_{x \in V(G)} d_x Z(G - \{x\})$$

Here $\mathrm{vol}(G)$ is defined to be twice the number of edges of G and $\tau(G)$ is the number of spanning trees of G.

Kemeny's constant is a very important invariant in random walk theory. Our formula also provides a fast algorithm for its calculation.

In Chapter 6, we study random walks on (edge-)weighted graphs. In fact, Chung-Yau invariants could also be defined on weighted graphs. We study restrictions on edge weights for a graph to be reversible.

2.0 RANDOM WALKS ON GRAPHS

2.1 GRAPH SPECTRA AND ELECTRIC NETWORKS

Unless otherwise specified, throughout the dissertation we assume $G = (V, E)$ to be undirected simple graph, namely for any two distinct vertices x, y there is at most one edge connecting x, y and there is no edge from x to itself. Denote by d_v the degree of a vertex v, i.e., the number of edges adjacent to v. The *volume* of G is $\mathrm{vol}(G) = \sum_{v \in V} d_v$. A *spanning tree* of G is a subgraph of G which itself is a tree (a connected graph without cycles) and contains all vertices of G. Let $\tau(G)$ be the number of spanning trees of G.

If the vertices of G are labeled by $\{1, 2, \ldots, |V|\}$, the *adjacency matrix* A of G is a square $|V| \times |V|$ matrix such that its element A_{ij} is one when there is an edge from i to j and zero otherwise. The *Laplacian* of G is the matrix $L = D - A$, where D is the diagonal matrix whose entries are the degree of the vertices and A is the adjacency matrix of G. For $x, y \in V$, $x \sim y$ denotes that they are adjacent vertices, i.e., there is an edge connecting x, y.

If G is connected with $n = |V|$ vertices, the eigenvalues of *Chung's normalized Laplacian* $\mathcal{L} = D^{-1/2} L D^{-1/2}$ can be labeled by (see [7])

$$0 = \lambda_1 < \lambda_2 \le \lambda_3 \le \cdots \le \lambda_n$$

with the corresponding orthonormal basis of eigenvectors $v_1, v_2, \cdots, v_n$. Note that both L and $\mathcal{L}$ are semi-positive definite. Let $v_i = (v_{i1}, \cdots, v_{in})^T$. Since v_i can also be regarded as a function on the set of vertices of G, we may determine v_i by specifying its values v_{ix} at all vertices x of G.

In particular, we have $v_{1x} = \sqrt{d_x / \mathrm{vol}(G)}, \forall x \in V$. This can be proved as follows: the summation of every row of L equals 0, hence $(1, 1, \cdots, 1)^T$ is an eigenvector of 0 for L. Let

v_1 be an eigenvector of 0 for $\mathcal{L}$. Then $\mathcal{L}v_1 = D^{-1/2}LD^{-1/2}v_1 = 0$ implies that $LD^{-1/2}v_1 = 0$. Setting $D^{-1/2}v_1 = (1, 1, \cdots, 1)^T$, so $v_1 = (\sqrt{d_1}, \cdots, \sqrt{d_n})^T$ is an eigenvector of 0 for $\mathcal{L}$. Normalized, $v_{1x} = \sqrt{d_x/\operatorname{vol}(G)}, \forall x \in V$.

A *random walk* on G is a time-reversible finite Markov chain $(X_0, X_1, \dots)$ with $X_i \in V$ that at each step it moves to a neighbor of the present vertex x with equal probability $1/d_x$. The *hitting time* $H(x, y)$ is the expected number of steps to reach y when started from x. The *cover time* $Cov_x(G)$ is the expected number of steps to visit all vertices of G when started from x. More precisely,

$$\begin{aligned} H(x,y) &= \mathbb{E}\left[\min\{t \geq 0 : X_t = y\} \mid X_0 = x\right], \\ Cov_x(G) &= \mathbb{E}\left[\min\{t \geq 0 : \cup_{i=0}^{t} X_i = V\} \mid X_0 = x\right]. \end{aligned}$$

We call $Cov(G) = \max_{x \in V} Cov_x(G)$ the cover time of G.

Chung and Yau [8] proved an explicit formula of $H(x, y)$ in terms of the discrete Green's function

$$H(x,y) = \operatorname{vol}(G)\left(\frac{\mathscr{G}(y,y)}{d_y} - \frac{\mathscr{G}(x,y)}{\sqrt{d_x d_y}}\right). \tag{2.1}$$

The discrete Green's function $\mathscr{G}$ is defined by

$$\mathscr{G}(x,y) = \sum_{k=2}^{n} \frac{1}{\lambda_k} v_{kx} v_{ky},$$

which is also uniquely determined by the equations

$$\mathscr{G}\mathcal{L} = \mathcal{L}\mathscr{G} = I - P_0, \qquad \mathscr{G}P_0 = 0, \qquad P_0 = v_1 v_1^T.$$

Hence (2.1) gives a connection of hitting times to spectra of $\mathcal{L}$,

$$H(x,y) = \operatorname{vol}(G) \sum_{k=2}^{n} \frac{1}{\lambda_k}\left(\frac{v_{ky}^2}{d_y} - \frac{v_{kx} v_{ky}}{\sqrt{d_x d_y}}\right). \tag{2.2}$$

Note that this is equivalent to the Lovász formula [16, Theorem 3.1], which used the spectra of $D^{-1/2}AD^{-1/2}$ instead of $\mathcal{L}$.

It is natural to regard a graph as an electrical network, where each edge has unit resistance. Chandra et al. [2] proved that the commute time $\kappa(x,y) := H(x,y) + H(y,x)$ can be expressed in terms of the effective resistance r_{xy} between x and y,

$$\kappa(x,y) = \mathrm{vol}(G) r_{xy}. \tag{2.3}$$

By using the reciprocity theorem of electrical networks, Tetali [23] proved a formula expressing $H(x,y)$ in terms of the effective resistance

$$H(x,y) = \frac{1}{2} \sum_{z \in V(G)} d_z (r_{xy} + r_{yz} - r_{xz}). \tag{2.4}$$

As remarked by Lovász [16, Corollary 4.2], one could use the method of electric networks to prove the following formula expressing the commute time in terms of the number of spanning trees

$$\kappa(x,y) = \mathrm{vol}(G) \frac{\tau(G/\{x,y\})}{\tau(G)}, \tag{2.5}$$

where $x \neq y \in V(G)$ and $G/\{x,y\}$ is the graph obtained from G by identifying x and y. Hence we have the following identity

$$r_{xy} = \frac{\tau(G/\{x,y\})}{\tau(G)}. \tag{2.6}$$

For a connected graph with n vertices and m edges, the *Kemeny's constant* $K(G)$ is defined by

$$K(G) = \frac{1}{\mathrm{vol}(G)} \sum_{y \in V(G)} d_y H(x,y), \tag{2.7}$$

which is known to be independent of $x \in V(G)$. Note that $\mathrm{vol}(G) = 2m$.

The *degree-Kirchhoff index* of graph G is defined by

$$Kf^*(G) = \frac{1}{2} \sum_{x,y \in V(G)} d_x d_y r_{xy}. \tag{2.8}$$

We have $Kf^*(G) = \mathrm{vol}(G) K(G)$ and $K(G) = \sum_{k=2}^{n} \frac{1}{\lambda_k}$, whose proofs can be found in [3, 10] and [16] respectively.

The traditional ways to calculate hitting times include the arguments by probability or first step analysis. More recently we have the methods through graph spectra, electric network and transition matrix technique.

1. Lovász's Formula

$$H(x,y) = \mathrm{vol}(G) \sum_{k=2}^{n} \frac{1}{\lambda_k} \left(\frac{v_{ky}^2}{d_y} - \frac{v_{kx} v_{ky}}{\sqrt{d_x d_y}} \right). \tag{2.9}$$

2. Tetali's Formula

$$H(x,y) = \frac{1}{2} \sum_{z \in V(G)} d_z (r_{xy} + r_{yz} - r_{xz}). \tag{2.10}$$

3. Transition matrix technique (see [18])

$$H(x,y) = \sum_{z=1}^{y-1} (I - Q)^{-1}_{xz}, \tag{2.11}$$

where Q is a $(n-1) \times (n-1)$ matrix derived by deleting nth row and nth column from the transition probability matrix $P = (p_{ij})_{1 \le i,j \le n}$, and I is the identity matrix.

2.2 HITTING AND COVER TIMES ON SPECIAL GRAPHS

Example 2.2.1. *Multiple ways to calculate hitting time of the complete graph K_n.*

Let's assume a complete graph on nodes $1, ..., n$. We may assume that we start from 1, and to find the hitting time, it suffices to determine $H(1,2)$.

1. Probability Approach. The probability that we first reach node 2 in the k-th step is $(\frac{n-2}{n-1})^{k-1} \frac{1}{n-1}$, and so the expected time from 1 to 2 is

$$H(1,2) = \sum_{k=1}^{\infty} k \left(\frac{n-2}{n-1} \right)^{k-1} \frac{1}{n-1} = n - 1. \tag{2.12}$$

2. First Step Analysis. We have the recursive relation:

$$H(1,2) = \frac{1}{d(1)} + \sum_{v \in V(K_n - \{1,2\})} \frac{1}{d(1)} [H(v,2) + 1], \tag{2.13}$$

where $d(1) = n - 1$ is the degree of 1. By symmetry, $H(v,2) = H(1,2)$ yields

$$H(1,2) = 1 + \frac{n-2}{n-1} H(1,2).$$

Hence $H(1,2) = n-1$.

3. Electric network approach. Let $r(1,2)$ represent the effective resistance between 1 and 2. It can be show that $r(1,2) = \frac{2}{n}$. By symmetry, we can contract all other $n-2$ vertices $K_n - \{1,2\}$ to a single vertex v to form an equivalent network with three vertices $\{1, v, 2\}$. There are $n-2$ edges between 1 and v so the resistance is $\frac{1}{n-2}$. Similarly, the resistance between v and 2 is also $\frac{1}{n-2}$. Therefore, the effective resistance between 1 and 2 is equal to

$$r(1,2) = \frac{1}{\frac{1}{1/(n-2)} + \frac{1}{1/(n-2)} + \frac{1}{1}} = \frac{2}{n}. \tag{2.14}$$

Thus by formula (2.10), $H(1,2) = n-1$.

4. Graph spectra approach. For complete graph, we have $\lambda_1 = 0$ and $\lambda_k = \frac{n}{n-1}$, for $k = 2, ..., n$. The corresponding orthonormal basis of eigenvectors $v_1, v_2, ..., v_n$ can be solved as follows:

$$\begin{bmatrix} \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{2}} & \cdots & 0 \\ \frac{1}{\sqrt{n}} & -\frac{1}{\sqrt{2}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\sqrt{n}} & 0 & \cdots & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{n}} & 0 & \cdots & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

Therefore by formula (2.9)

$$H(1,2) = n(n-1)\sum_{k=2}^{n} \frac{n-1}{n} \cdot \frac{1}{n-1}(v_{k2}^2 - v_{k1}v_{k2}) = n-1.$$

5. Transition matrix approach (we follow [18]). For complete graph, we have

$$Q = \begin{bmatrix} 0 & \frac{1}{n-1} & \cdots & \frac{1}{n-1} & \frac{1}{n-1} \\ \frac{1}{n-1} & 0 & \frac{1}{n-1} & \cdots & \frac{1}{n-1} \\ \frac{1}{n-1} & \frac{1}{n-1} & 0 & \cdots & \frac{1}{n-1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{1}{n-1} & \frac{1}{n-1} & \frac{1}{n-1} & \cdots & 0 \end{bmatrix}$$

and

$$(I-Q)^{-1} = \frac{n-1}{n}\begin{bmatrix} 2 & 1 & \cdots & 1 & 1 \\ 1 & 2 & 1 & \cdots & 1 \\ 1 & 1 & 2 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 1 & 1 & \cdots & 2 \end{bmatrix}$$

Hence by formula (2.11) we obtain

$$H(1,2) = \frac{n-1}{n}(2+n-2) = n-1.$$

Example 2.2.2. *Calculate the Kemeny's constant of the complete graph K_n.*

For complete graph K_n, we have $\mathrm{vol}(K_n) = n(n-1)$, $d_y = n-1$ and $H(x,y) = n-1$ for $x, y \in V(K_n)$. Hence, by (2.7) we have

$$K(K_n) = n-1.$$

Example 2.2.3. *Calculate the degree-Kirchhoff index of the complete graph K_n.*

For complete graph, the effective resistance $r_{xy} = 2/n$ for $x, y \in V(K_n)$ by Example 2.2.1, method 3. Therefore, by (2.8) the *degree-Kirchhoff index*

$$Kf^*(K_n) = \frac{1}{2}n^2(n-1)^2 \cdot \frac{2}{n} = n(n-1)^2.$$

Example 2.2.4. *Calculate cover time of the complete graph K_n.*

We follow [16]. The cover time of graph G is defined by

$$Cov(G) = \max_{x\in V(G)} Cov_x(G), \tag{2.15}$$

where $Cov_x(G)$ is the expected number of steps to visit all vertices of G when started from x. Let τ_i denote the number of steps taken so that i distinct vertices been visited for the first time. So we have $\tau_1 = 0 < \tau_2 = 1 < \tau_3 < \cdots < \tau_n$. Now $\tau_{i+1} - \tau_i$ is the number of steps needed to first time visit another new vertex other than the existing i vertices. For complete graph K_n, $\tau_{i+1} - \tau_i$ follows the geometric distribution with probability $p = \frac{n-i}{n-1}$. Hence

$$E(\tau_{i+1} - \tau_i) = \frac{1}{p} = \frac{n-1}{n-i}, \tag{2.16}$$

for $i = 1, 2, \ldots, n$. Therefore, the cover time of K_n can be calculated as

$$E(\tau_n) = \sum_{i=1}^{n-1} E(\tau_{i+1} - \tau_i) = (n-1)\sum_{i=1}^{n-1} \frac{1}{i} \sim (n-1)\log(n-1), \tag{2.17}$$

as $n \to \infty$.

Example 2.2.5. *Multiple ways to calculate hitting time $H(i,k)$ of the path P_n on n vertices, where $0 \le i < k \le n-1$.*

1. First Step Analysis. We have the recursive relation:

$$H(i,k) = 1 + \frac{1}{2}(H(i-1,k) + H(i+1,k)), 1 \le i \le k-1. \tag{2.18}$$

and $H(0,k) = 1 + H(1,k)$. This implies $H(i,k) - H(i-1,k) = 2 + H(i+1,k) - H(i,k)$ for $1 \le i \le k-1$. Summing up both sides we obtain $H(k-1,k) = 2k-1$. Now for hitting time $H(i,k)$, we have $H(i,k) = H(i,k-1) + H(k-1,k) = H(i,k-1) + 2k - 1$. Therefore,

$$H(i,k) = (2i+1) + (2i+3) + ... + (2k-1) = k^2 - i^2.$$

2. Electric network. For path, we know $d_0 = d_{n-1} = 1$ and $d_j = 2$ for $1 \le j \le n-2$. r_{kj} represents the resistance between k and j, which is $|k-j|$. Similarly, $r_{ij} = |i-j|$ and $r_{ik} = k - i$. Therefore, by (2.10)

$$\begin{aligned} H(i,k) &= \frac{1}{2}(k-i)\cdot 2(n-1) + \frac{1}{2}\sum_{j=0}^{n-1}(|k-j| - |i-j|)\cdot d_j \\ &= (k-i)(n-1) + \sum_{j=1}^{i}(k-i) + \sum_{j=i+1}^{k-1}(k+i-2j) + \sum_{j=k}^{n-2}(i-k) \\ &= (k-i)[n-1+i-(n-k-1)] \\ &= k^2 - i^2. \end{aligned}$$

3. Transition matrix technique (we follow [18]). For path, we have

$$Q = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & \cdots & 0 & 0 \\ 0 & \frac{1}{2} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{1}{2} & 0 \end{bmatrix}$$

and

$$(I-Q)^{-1}=\begin{bmatrix} n-1 & 2(n-2) & 2(n-3) & \cdots & 6 & 4 & 2 \\ n-2 & 2(n-2) & 2(n-3) & \cdots & 6 & 4 & 2 \\ n-3 & 2(n-3) & 2(n-3) & \cdots & 6 & 4 & 2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 3 & 6 & 6 & \cdots & 6 & 4 & 2 \\ 2 & 4 & 4 & \cdots & 4 & 4 & 2 \\ 1 & 2 & 2 & \cdots & 2 & 2 & 2 \end{bmatrix}$$

Therefore, by (2.11), we get

$$\begin{aligned} H(x,n) &= \sum_{z=1}^{n-1}(I-Q)^{-1}_{x,z} \\ &= 2(1+2+\cdots+n-x-1)+(2x-1)(n-x) \\ &= (n+x-2)(n-x) \end{aligned}$$

take $x=i+1$ and $n=k+1$, we have $H(i,k)=(i+k)(k-i)=k^2-i^2$.

Example 2.2.6. *Calculate the Kemeny's constant of the path P_n.*

In (2.7), taking $x=0$, we have

$$\begin{aligned} K_0(P_n) &= \frac{1}{2(n-1)}\left[\sum_{y=1}^{n-2}2y^2+(n-1)^2\right] \\ &= \frac{1}{2(n-1)}\left[\frac{1}{3}(n-2)(n-1)(2n-3)+(n-1)^2\right] \\ &= \frac{1}{6}(n-2)(2n-3)+\frac{1}{2}(n-1) \\ &= \frac{1}{6}(2n^2-4n+3). \end{aligned}$$

Example 2.2.7. *Calculate the degree-Kirchhoff index of the path P_n.*

For path, the effective resistance $r_{xy}=|x-y|$ for $0 <= x, y \leq n-1$. By Formula (2.8), we have

$$Kf^*(P_n) = \sum_{0\leq i<j\leq n-1} d_i d_j (j-i)$$

$$
\begin{aligned}
&= \sum_{i=0}^{n-2} d_i \sum_{j=i+1}^{n-1} d_j(j-i) \\
&= \sum_{i=0}^{n-2} d_i \sum_{j=1}^{n-i-1} d_{j+i} \cdot j \\
&= \sum_{j=1}^{n-1} d_j \cdot j + d_{n-2}d_{n-1} + 2\sum_{i=1}^{n-3}\sum_{j=1}^{n-i-1} d_{j+i} \cdot j \\
&= (n-1)^2 + 2 + 2\sum_{i=1}^{n-3}\left(\sum_{j=1}^{n-2-i} 2j + (n-1-i)\right) \\
&= (n-1)^2 + 2 + n(n-3) + 2\sum_{i=1}^{n-3}(n-1-i)(n-2-i) \\
&= (2n-3)(n-1) + \frac{2}{3}(n-3)(n-2)(n-1) \\
&= \frac{1}{3}(n-1)(2n^2-4n+3).
\end{aligned}
$$

Example 2.2.8. *Calculate cover time of the path P_n.*

Let $0 \le k \le n-1$. To cover P_n, the walk need to first reach 0 or $n-1$, then walk to the other end. We can glue vertices 0 and $n-1$ into a new vertex s, and form a new cycle C_{n-1} on $n-1$ vertices. Then the hitting time from k to either 0 or $n-1$ is equal to the hitting time from k to s in C_{n-1}, which is $k(n-k-1)$. Hence $Cov_k(P_n) = k(n-k-1) + (n-1)^2$. If $k = n-k-1$, which implies that $k = \frac{1}{2}(n-1)$, then $\max_{k \in V(P_n)} Cov_k(P_n)$ happens. Therefore,

$$
Cov(P_n) = \begin{cases} \frac{1}{4}n(n-2) + (n-1)^2 & \text{if } n \text{ is even,} \\ \frac{1}{4}n(n-1) + (n-1)^2 & \text{if } n \text{ is odd.} \end{cases}
$$

The following lemma and its corollary will be used in calculating hitting times of the cycle by transition matrix technique.

Lemma 2.2.1 (Sherman-Morrison)**.** *Suppose $A \in \mathbb{R}^{n\times n}$ is an invertible square matrix and $u, v \in \mathbb{R}^n$ are column vectors. Then $A + uv^T$ is invertible if and only if $1 + v^T A^{-1} u \neq 0$. In this case,*

$$
\left(A + uv^T\right)^{-1} = A^{-1} - \frac{A^{-1}uv^TA^{-1}}{1 + v^TA^{-1}u}. \tag{2.19}
$$

The above Lemma 2.2.1 implies the following.

Corollary 2.2.2. *If A and $A+B$ are invertible, and $\operatorname{rank}(B) = 1$. Then $\operatorname{tr}(BA^{-1}) \neq -1$ and*

$$(A+B)^{-1} = A^{-1} - \frac{A^{-1}BA^{-1}}{1+\operatorname{tr}(BA^{-1})}. \tag{2.20}$$

Proof. Since B has rank 1, we can write $B = uv^T$, where u, $v \in \mathbb{R}^n$ are column vectors. Then $\operatorname{tr}(BA^{-1}) = \operatorname{tr}(A^{-1}B) = \operatorname{tr}(A^{-1}uv^T) = v^T A^{-1} u$. By A and $A+B$ are invertible, the corollary follows directly from Lemma 2.2.1. □

Example 2.2.9. *Multiple ways to calculate hitting time $H(i,j)$ of the cycle C_n on n vertices, where $1 \leq i < j \leq n$.*

1. First step analysis. We have

$$H(i,j) = 1 + \frac{1}{2}H(i-1,j) + \frac{1}{2}H(i+1,j)$$

holds for all $1 \leq i < j \leq n$. The corresponding $n \times n$ coefficient matrix

$$A = \begin{bmatrix} -2 & 1 & & & & 1 \\ 1 & -2 & 1 & & & \\ & & \ddots & & & \\ & & & -2 & & \\ & & & \ddots & & \\ 1 & & & & 1 & -2 \end{bmatrix}$$

Since the sum of every row and the sum of every column are equal to 0, then all cofactors of A are equal, so the rank of A is $n-1$. Hence the dimension of the null space is 1. We can check that $H(i,j) = (j-i)(n-j-i)$ satisfy the above recursion. So, $H(i,j) = (j-i)(n-j+i)+c$, here c is a constant number. Let $i=j$, then $c = H(j,j) = 0$. Therefore, $H(i,j) = (j-i)(n-j+i)$.

2. Electric network approach. For cycle, $d_k = 2$ and

$$r_{ij} = \frac{1}{1/|j-i| + 1/(n-|j-i|)} = \frac{1}{n}(|j-i|)(n-|j-i|). \tag{2.21}$$

In (2.10), by symmetry we have $\sum_{k=1}^{n} r_{ik} - r_{jk} = 0$, yielding $H(i,j) = |j-i| \cdot (n-|j-i|)$.

3. Graph spectra approach. The cycle C_n has eigenvalues $\lambda_k = 1 - \cos(\frac{2\pi k}{n})$, for $k = 1, ..., n-1$. Note that for $1 \leq k \leq \frac{n}{2}$, $\lambda_k = \lambda_{n-k}$. The eigenvector of $\lambda_1 = 0$ is $(\frac{1}{\sqrt{n}}, \cdots, \frac{1}{\sqrt{n}})^T$. For $1 \leq k \leq \frac{n}{2}$, the eigenvectors of λ_k are

$$x_k(v) = \sin\left(\frac{2\pi k v}{n}\right), \quad y_k(v) = \cos\left(\frac{2\pi k v}{n}\right), \tag{2.22}$$

where $v = 1, ..., n$. When n is even, $x_{n/2}$ is zero vector. So the only eigenvector for $\lambda_{n/2}$ is $y_{n/2}$. Namely $\lambda_{n/2}$ is simple. From the above formulas of eigenvalues and eigenvectors of C_n, we could apply Lovász formula to get hitting time on C_n, but the computation is long and tedious. We omit the details.

4. Transition matrix approach. For the cycle C_n on n vertices, the transition matrix is

$$Q = \begin{bmatrix} 0 & \frac{1}{2} & 0 & \cdots & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & \cdots & 0 & 0 \\ 0 & \frac{1}{2} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{1}{2} & 0 \end{bmatrix}$$

and

$$(I-Q)^{-1} = \begin{bmatrix} n-1 & 2(n-2) & 2(n-3) & \cdots & 6 & 4 & 2 \\ n-2 & 2(n-2) & 2(n-3) & \cdots & 6 & 4 & 2 \\ n-3 & 2(n-3) & 2(n-3) & \cdots & 6 & 4 & 2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 3 & 6 & 6 & \cdots & 6 & 4 & 2 \\ 2 & 4 & 4 & \cdots & 4 & 4 & 2 \\ 1 & 2 & 2 & \cdots & 2 & 2 & 2 \end{bmatrix}$$

$$- \frac{1}{n} \begin{bmatrix} (n-2)(n-1) & 2(n-2)(n-1) & 2(n-3)(n-1) & \cdots & 4(n-1) & 2(n-1) \\ (n-2)(n-2) & 2(n-2)(n-2) & 2(n-3)(n-2) & \cdots & 4(n-2) & 2(n-2) \\ (n-2)(n-3) & 2(n-2)(n-3) & 2(n-3)(n-2) & \cdots & 4(n-3) & 2(n-3) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ (n-2)\times 3 & 2(n-2)\times 3 & 2(n-3)\times 3 & \cdots & 4\times 3 & 2\times 3 \\ (n-2)\times 2 & 2(n-1)\times 2 & 2(n-3)\times 2 & \cdots & 4\times 2 & 2\times 2 \\ n-2 & 2(n-2) & 2(n-3) & \cdots & 4 & 2 \end{bmatrix}$$

The derivation of $(I-Q)^{-1}$ for cycles used the corresponding formula of $(I-Q)^{-1}$ for paths and Corollary 2.2.2. By (2.11), it is not difficult to get $H(i,j)=(j-i)(n-j+i)$ for all $1\le i<j\le n$.

Example 2.2.10. *Calculate the Kemeny's constant of the cycle C_n.*

Take $x=1$ in (2.7), we have

$$\begin{aligned}
K(C_n) &= \frac{1}{2n}\sum_{i=2}^{n} 2(i-1)(n-i+1)\\
&= \frac{1}{2n}\sum_{i=1}^{n-1}\left[n^2-i^2-(n-i)^2\right]\\
&= \frac{1}{2n}(n-1)n^2-\frac{1}{n}\sum_{i=1}^{n-1} i^2\\
&= \frac{1}{6}(n^2-1)
\end{aligned}$$

Example 2.2.11. *Calculate the degree-Kirchhoff index of the cycle C_n.*

By symmetry and plug (2.21) into (2.8), we have

$$\begin{aligned}
Kf^*(C_n) &= 4\sum_{1\le i<j\le n}\frac{1}{n}(j-i)(n-j+i)\\
&= 4\sum_{i=1}^{n-1}\sum_{j-i=1}^{n-i}\frac{1}{n}(j-i)(n-j+i)\\
&= 4\sum_{i=1}^{n-1}\sum_{k=1}^{i}\frac{1}{n}k(n-k)\\
&= 4\sum_{k=1}^{n-1}\frac{1}{n}k^2(n-k)\\
&= \frac{2}{3}n(n-1)(2n-1)-\frac{1}{n}(n-1)^2n^2\\
&= \frac{1}{3}n(n^2-1).
\end{aligned}$$

Note that $Kf^*(C_n)=2n\cdot K(C_n)=\mathrm{vol}(C_n)\cdot K(C_n)$.

Example 2.2.12. *Calculate cover time of the cycle C_n.*

Let $1 \leq k \leq n-1$. Assume that the walker has just visited the k-th vertex and is now at the vertex i. We contract all the $n-k$ vertices that have not been visited yet into a single vertex j. This forms a new cycle C_{k+1} with $k+1$ vertices. Hence the hitting time from i to j in C_{k+1} is equal to k, which is the expected number of steps for the walker to reach $(k+1)$-th vertex. The cover time of the cycle C_n is therefore:

$$Cov(C_n) = \sum_{k=1}^{n-1} k = \frac{1}{2} n(n-1).$$

3.0 CHUNG-YAU INVARIANTS AND DISCRETE GREEN'S FUNCTION

The discrete Green's function was defined in Chapter 2. In view of the connections to random walks, it is more convenient to use the following normalized discrete Green's function $\mathcal{G}$,

$$\mathcal{G}(x,y) = \frac{\mathscr{G}(x,y)}{\sqrt{d_x d_y}}. \tag{3.1}$$

Both $\mathscr{G}$ and $\mathcal{G}$ are symmetric matrices.

Chung and Yau [8] proved the following formulas of $H(x,y)$ in terms of discrete Green's function and vice versa.

Theorem 3.0.1. (Chung-Yau) *On a connected graph* Γ*, the hitting time* $H(x,y)$ *and discrete Green's function* $\mathcal{G}(x,y)$ *satisfy*

$$H(x,y) = \mathrm{vol}(\Gamma)\big(\mathcal{G}(y,y) - \mathcal{G}(x,y)\big), \tag{3.2}$$

$$\mathcal{G}(x,y) = -\frac{1}{\mathrm{vol}(\Gamma)}H(x,y) + \frac{1}{\mathrm{vol}(\Gamma)^2}\sum_{z\in V(\Gamma)} d_z H(z,y). \tag{3.3}$$

In the remaining of this chapter, we follow the expositions of [24] (Sections 3.1 and 3.2) and [25] (Section 3.3). We try to supply with alternative proofs (e.g., Theorems 3.3.4, 3.3.5, 3.3.6, 3.3.8) or more details (e.g., Lemma 3.1.2). Some results (e.g., Theorem 3.1.14) are improved.

3.1 CHUNG-YAU INVARIANTS OF VERTEX-WEIGHTED GRAPHS

First we give a brief summary of the Chung-Yau invariants before going into a detailed study. The Chung-Yau invariants consist of R and Z invariants, which are computationally efficient as they are simply the determinants of submatrices of a given matrix. The recursive formula of the R-invariant can be used to get closed formulas of the number of spanning trees of graphs. It could be regarded as a recursive version of Kirchhoff's Matrix-Tree Theorem and is sometimes more effective as it does not require knowing the eigenvalues of the graph. The Z-invariant is determined by R-invariant and we will apply it to study graphs with symmetric hitting times.

The famous Kirchhoff's Matrix-Tree Theorem relates the number of spanning trees of a graph G with the spectra of its Laplacian L or normalized Laplacian $\mathcal{L}$. The following version of Kirchhoff Matrix-Tree Theorem can be found in [7].

Theorem 3.1.1. *For a graph $\Gamma = (V, E)$ whose eigenvalues of $\mathcal{L}$ are given by $0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_n$, we have*

$$\prod_{k=2}^{n} \lambda_k = \frac{\mathrm{vol}(\Gamma)\tau(\Gamma)}{\prod_{v \in V} d_v},$$

where $\tau(\Gamma)$ is the number of spanning trees of Γ.

The following lemma and corollary are the key techniques about a combinatorial interpretation of the matrix determinant which is an alternating summation over permutations of n elements. They should be considered well-known results in linear algebra.

Lemma 3.1.2. *Given a $n \times n$ matrix $M = (a_{ij})$, we can define a digraph G of n vertices, having an arc from i to j of weight a_{ij} if and only if $a_{ij} \neq 0$. A spanning linear subgraph Δ of G has the property that each vertex has exactly one outgoing arc and one incoming arc. Let k be the number of connected components of Δ, the weight of Δ is defined to be $(-1)^{n+k}$ times the product of the weights of all its arcs. Then $\det M$ is equal to the sum of the weights of all spanning linear subgraphs of G.*

Proof. Recall the following formula of the determinant of an $n \times n$ matrix $M = (a_{ij})$.

$$\det M = \sum_{\sigma \in S_n} \left(\mathrm{sgn}(\sigma) \prod_{i=1}^{n} a_{i,\sigma(i)} \right).$$

Here the sum is computed over all permutations σ of $\{1, 2, \ldots, n\}$ and $\mathrm{sgn}(\sigma)$ denotes the signature of σ, namely $+1$ for even permutation and -1 for odd permutation.

Fix a $\sigma \in S_n$. Among vertices $\{1, 2, \ldots, n\}$, for each $1 \leq i \leq n$, we draw an arc from i to $\sigma(i)$. Then we get a linear subgraph Δ_σ of G defined in the corollary. We see that $\prod_{i=1}^{n} a_{i,\sigma(i)}$ is just the weight of Δ_σ up to sign. The sign is easily seen to be $(-1)^{n+k}$ where k is the number of connected components of Δ_σ. Finally when σ runs over S_n, we exhaust exactly all linear subgraphs of G. □

The above Lemma 3.1.2 implies the following.

Corollary 3.1.3. *We use the same notation in the above lemma. Let $1 \leq i \neq j \leq n$. Let M_{ij} be the matrix obtained by deleting the i-th column and the j-th row of M. Then the (j, i) minor* $\det M_{ij}$ *is equal to the sum of the weights of all spanning subgraphs of G whose components consist of a directed path from i to j and some linear subgraphs.*

Proof. Without loss of generality, we may take $i = 1$ and $j = 2$, then the assertion follows easily from Lemma 3.1.2. □

Next we are going to find an explicit formula of discrete Green's function in terms of the Chung-Yau invariants. Since discrete Green's function is symmetric, we will adapt Lemma 3.1.2 and Corollary 3.1.3 to the setting of symmetric matrices and associated undirected weighted graphs.

For an undirected simple graph Γ, we may associate a directed graph $\widetilde{\Gamma}$ with the same vertex set as Γ and an arc $uv \in E(\widetilde{\Gamma})$ if and only if $u = v$ or $u \sim v$ in Γ. Denote by $\mathscr{D}(\Gamma)$ the set consisting of all spanning subgraphs Δ of Γ such that each component of Δ is either a vertex, an edge or a cycle. A vertex and an edge may be regarded as 0-cycle and 1-cycle respectively. $\mathscr{D}(\Gamma)$ is the undirected counterpart of spanning linear subgraphs of $\widetilde{\Gamma}$. The only difference is that an undirected k-cycle ($k \geq 3$) has two orientations: clockwise or counterclockwise.

Let $\Delta \in \mathscr{D}(\Gamma)$. We denote by $\alpha_k(\Delta)$ the number of components of Δ with no less than k vertices and $\mathcal{I}(\Delta)$ the set of single-vertex components of Δ. If $(x, y) \in E(\Delta)$ is an edge, then we define $e(x, y)$ by

$$e(x,y) = \begin{cases} 2 & \text{if } (x,y) \text{ is a component of } \Delta, \\ 1 & \text{otherwise.} \end{cases}$$

A *vertex-weighted graph* is an undirected graph Γ in which each vertex is assigned a weight $w : V(\Gamma) \to \mathbb{R}$.

Definition 3.1.1. *The two Chung-Yau invariants for a vertex-weighted graph (Γ, w) are defined as follows:*

$$\begin{aligned} R(\Gamma; w) &= \sum_{\Delta \in \mathscr{D}(\Gamma)} (-1)^{\alpha_2(\Delta)} 2^{\alpha_3(\Delta)} \prod_{v \in \mathcal{I}(\Delta)} w_v, \\ Z(\Gamma; w) &= \sum_{\Delta \in \mathscr{D}(\Gamma)} (-1)^{\alpha_2(\Delta)} 2^{\alpha_3(\Delta)} \prod_{v \in \mathcal{I}(\Delta)} w_v \Big(\sum_{v \in \mathcal{I}(\Delta)} w_v - \sum_{(x,y) \in E(\Delta)} e(x,y) w_x w_y \Big) \\ &\quad + \sum_{\substack{x,y \in V(\Gamma) \\ x \nsim y}} \sum_{P \in \mathscr{P}_\Gamma(x,y)} w_x w_y R(\Gamma - P; w), \end{aligned}$$

where $\mathscr{P}_\Gamma(x, y)$ is the set of all simple paths (with no repeated vertices) connecting x and y in Γ. We assume that $\mathscr{P}_\Gamma(x, x)$ consists of the trivial path $\{x\}$ only. Here $\Gamma - P$ means the graph obtained from Γ by removing the vertices of P together with incident edges.

By convention, for empty graph $\emptyset$, we have $R(\emptyset; w) = 1$ and $Z(\emptyset; w) = 0$.

Lemma 3.1.4. *(1) Let Γ be the single vertex pt with weight a. Then*

$$R(pt; a) = a, \qquad Z(pt; a) = a^2. \tag{3.4}$$

(2) Let P_2 be the two-vertex path with weight $[a, b]$. Then

$$R(P_2; [a,b]) = ab - 1, \qquad Z(P_2; [a,b]) = ab(a + b + 2). \tag{3.5}$$

Proof. For a single vertex graph *pt*, the set $\mathscr{D}(pt)$ has the loop at *pt* as its unique element. For P_2, the set $\mathscr{D}(P_2)$ has two elements, namely the 2 loops at each vertex and the 2-cycle. Then the lemma follows easily. □

Theorem 3.1.5. *Let s be a formal variable. If we denote by B_s the following matrix*

$$B_s(x,y) = \begin{cases} w_x^2 s + w_x & \text{if } x = y, \\ w_x w_y s - 1 & \text{if } x \sim y, \\ w_x w_y s & \text{otherwise,} \end{cases} \tag{3.6}$$

then we have $\det B_s = R(\Gamma; w) + Z(\Gamma; w) \cdot s$.

Proof. It is not difficult to see that $R(\Gamma; w)$ is a weighted counting of spanning linear subgraphs of $\widetilde{\Gamma}$ and $Z(\Gamma; w)$ is a weighted counting of all spanning subgraphs of $\widetilde{\Gamma}$ that can be obtained by removing an edge (keeping the end vertices) from some spanning linear subgraph of $\widetilde{\Gamma}$. Then apply Lemma 3.1.2. Also the terms in $\det B_s$ with degree of $s \geq 2$ all vanish. □

Remark 3.1.6. *In fact, in this paper, we are mainly interested in the Chung-Yau invariants of a very special kind of vertex-weighted graph. Namely we fix an undirected graph Γ, the weight w_x at $x \in V(\Gamma)$ will be the degree of x in the ambient graph Γ. So we may assume $d_x \leq w_x \in \mathbb{Z}$. If $w_x = d_x$, $\forall x \in V(\Gamma)$, this weight function will be denoted by d_Γ. In this way, we defined Chung-Yau invariants for all induced subgraphs of Γ.*

Below we present some basic properties of Chung-Yau invariants.

Lemma 3.1.7. *If Γ has k connected components $\Gamma_1, \dots, \Gamma_k$, then*

$$R(\Gamma; w) = \prod_{i=1}^{k} R(\Gamma_i; w), \tag{3.7}$$

$$Z(\Gamma; w) = \sum_{i=1}^{k} Z(\Gamma_i; w) \prod_{\substack{j=1 \\ j \neq i}}^{k} R(\Gamma_j; w). \tag{3.8}$$

Proof. Both identities follow from their definitions or Theorem 3.1.5. □

The following two lemmas give recursive relations of Chung-Yau invariants.

Lemma 3.1.8. *Fix a vertex $x \in V(\Gamma)$ and denote by $\mathscr{C}(\Gamma)$ the set of all cycles in Γ, we have the following effective recursive formulas for computing $R(\Gamma; w)$ and $Z(\Gamma; w)$.*

$$R(\Gamma; w) = w_x R(\Gamma - x; w) - \sum_{\substack{y \in V(\Gamma) \\ y \sim x}} R(\Gamma - \{x, y\}; w) - 2 \sum_{\substack{C \in \mathscr{C}(\Gamma) \\ x \in C}} R(\Gamma - C; w), \tag{3.9}$$

$$\begin{aligned} Z(\Gamma; w) = {} & w_x Z(\Gamma - x; w) - \sum_{\substack{y \in V(\Gamma) \\ y \sim x}} Z(\Gamma - \{x, y\}; w) - 2 \sum_{\substack{C \in \mathscr{C}(\Gamma) \\ x \in C}} Z(\Gamma - C; w) \\ & + w_x^2 R(\Gamma - x; w) + \sum_{\substack{u, v \in V(\Gamma) \\ u \neq v}} \sum_{\substack{P_1 \in \mathscr{P}_\Gamma(x,u) \\ P_2 \in \mathscr{P}_\Gamma(x,v) \\ P_1 \cap P_2 = x}} w_u w_v R(\Gamma - \{P_1, P_2\}; w). \end{aligned} \tag{3.10}$$

Proof. Fix a vertex x, any spanning linear subgraph of Γ consists of a cycle C containing x, and a spanning linear subgraph of $\Gamma - C$. Then these formulas follow from the definitions and Lemma 3.1.2. □

Lemma 3.1.9. *Fix a vertex $x \in V(\Gamma)$, we have*

$$R(\Gamma; w) = w_x R(\Gamma - x; w) - \sum_{\substack{y \in V(\Gamma) \\ y \sim x}} \sum_{P \in \mathscr{P}_\Gamma(x,y)} R(\Gamma - P; w), \tag{3.11}$$

$$\begin{aligned} Z(\Gamma; w) = {} & w_x Z(\Gamma - x; w) - \sum_{\substack{y \in V(\Gamma) \\ y \sim x}} \sum_{P \in \mathscr{P}_\Gamma(x,y)} Z(\Gamma - P; w) \\ & + w_x^2 R(\Gamma - x; w) + \sum_{\substack{u, v \in V(\Gamma) \\ u \neq v}} \sum_{\substack{P_1 \in \mathscr{P}_\Gamma(x,u) \\ P_2 \in \mathscr{P}_\Gamma(x,v) \\ P_1 \cap P_2 = x}} w_u w_v R(\Gamma - \{P_1, P_2\}; w). \end{aligned} \tag{3.12}$$

Proof. Note that a cycle at $x \in V(\Gamma)$ is just a path from x to one of its neighbors y followed by the edge yx. So the lemma follows from Lemma 3.1.8. □

The next lemma shows that Z invariant is determined by the R invariant.

Lemma 3.1.10. *We have*

$$Z(\Gamma; w) = \sum_{x, y \in V(\Gamma)} \sum_{P \in \mathscr{P}_\Gamma(x,y)} w_x w_y R(\Gamma - P; w). \tag{3.13}$$

Proof. Both identities follow from the definitions of Chung-Yau invariants or Theorem 3.1.5.
□

Recall the following well-known results from linear algebra.

Lemma 3.1.11. *Let M be an $n \times n$ matrix whose rows and columns all sum to zero. Then all cofactors $(-1)^{i+j}\det(M_{ij})$ of M are equal.*

Lemma 3.1.12. *Let Γ be a connected graph with Laplacian matrix L. Let L' denote the matrix obtained by deleting the first row and column from L. Then:*

$$\tau(\Gamma) = \det(L').$$

Lemma 3.1.12 is a version of Kirchhoff matrix tree theorem. The R invariant is closely related to the numbers of spanning trees.

Lemma 3.1.13. *Let Γ be a connected graph. For any $x, y \in V(\Gamma)$, we have*

$$R(\Gamma - \{x\}; d_\Gamma) = \sum_{P \in \mathscr{P}_\Gamma(x,y)} R(\Gamma - P; d_\Gamma) = \tau(\Gamma). \tag{3.14}$$

Proof. Recall that the Laplacian L of Γ is given by

$$L(x,y) = \begin{cases} d_x & \text{if } x = y, \\ -1 & \text{if } x \sim y, \\ 0 & \text{otherwise.} \end{cases}$$

In fact, from Theorem 3.1.5, we have that for any subgraph S of Γ, $R(\Gamma - \{S\}; d_\Gamma)$ is equal to $\det(L_S)$ here L_S is the submatrix of Laplacian L obtained by deleting rows and columns corresponding to vertices of S. Hence $R(\Gamma - \{S\}; d_\Gamma) = R(\Gamma/S)$ where Γ/S is the graph obtained from Γ by contracting S to a vertex. In particular, $R(\Gamma - \{x\}; d_\Gamma) = \det(L_{xx}) = \tau(G)$ and $\sum_{P \in \mathscr{P}_\Gamma(x,y)} R(\Gamma - P; d_\Gamma) = -\det(L_{xy}) = \tau(G)$. So (3.14) is proved. □

Explicit formulas of $R(\Gamma; w)$ for certain special graphs with arbitrary weights can be found in the appendix of [24].

Now we come to prove an explicit formula for discrete Green's function in terms of Chung-Yau invariants.

Theorem 3.1.14. *Let Γ be a connected graph and $x, y \in V(\Gamma)$. Then*

$$\mathcal{G}(x,y) = \frac{1}{\operatorname{vol}(\Gamma)^2\tau(\Gamma)} \left(\sum_{P \in \mathscr{P}_\Gamma(x,y)} Z(\Gamma - P; d_\Gamma) - \sum_{\substack{u,v \in V(\Gamma)\\ u \neq v}} \sum_{\substack{P_1 \in \mathscr{P}_\Gamma(x,u)\\ P_2 \in \mathscr{P}_\Gamma(y,v)\\ P_1 \cap P_2 = \emptyset}} d_u d_v R(\Gamma - \{P_1, P_2\}; d_\Gamma) \right). \quad (3.15)$$

In particular, when $x = y$,

$$\mathcal{G}(x,x) = \frac{Z(\Gamma - \{x\}; d_\Gamma)}{\operatorname{vol}(\Gamma)^2\tau(\Gamma)}. \quad (3.16)$$

Proof. We follow the proof in [24]. By definition,

$$\mathscr{G}(x,y) = \sum_{i=2}^{n} \frac{1}{\lambda_i}\phi_i(x)\phi_i(y), \quad \forall x, y \in V(\Gamma),$$

which is equivalent to $\mathscr{G} = \Phi \operatorname{diag}[0, 1/\lambda_2, \ldots, 1/\lambda_n]\Phi^T$, where $\Phi = (\phi_1, \ldots, \phi_n)$ is an $n \times n$ orthogonal matrix. Since $\phi_1 = (\sqrt{d_1/\operatorname{vol}(\Gamma)}, \ldots, \sqrt{d_n/\operatorname{vol}(\Gamma)})^T$, we have

$$D^{1/2}JD^{1/2} = \Phi \operatorname{diag}[\operatorname{vol}(\Gamma), 0, \ldots, 0]\Phi^T,$$

where J is the $n \times n$ matrix with all entries equal to 1. From $\Phi^T\mathcal{L}\Phi = \operatorname{diag}[0, \lambda_2, \ldots, \lambda_n]$, we get

$$\mathscr{G} = (\mathcal{L} + D^{1/2}JD^{1/2})^{-1} - \frac{1}{\operatorname{vol}(\Gamma)^2}D^{1/2}JD^{1/2}.$$

In terms of $\mathcal{G}$, we have

$$\mathcal{G} = D^{-1/2}\mathscr{G}D^{-1/2} = D^{-1}M^{-1}D^{-1} - \frac{1}{\operatorname{vol}(\Gamma)^2}J, \quad (3.17)$$

where $M = M_1 = D^{-1/2}(\mathcal{L} + D^{1/2}JD^{1/2})D^{-1/2}$ is given by

$$M_s(x,y) = \begin{cases} s + 1/d_x & \text{if } x = y, \\ s - 1/d_x d_y & \text{if } x \sim y, \\ s & \text{otherwise.} \end{cases} \quad (3.18)$$

By definition,

$$\left(\prod_{x \in V(\Gamma)} d_x \right)^2 \det M_s = R(\Gamma; d_\Gamma) + Z(\Gamma; d_\Gamma) \cdot s. \quad (3.19)$$

Moreover, by the Matrix-Tree Theorem 3.1.1, we have

$$\det M = \frac{\mathrm{vol}(\Gamma)\prod_{i=2}^{n}\lambda_i}{\prod_{x\in V(\Gamma)} d_x} = \frac{\mathrm{vol}(\Gamma)^2\tau(\Gamma)}{(\prod_{x\in V(\Gamma)} d_x)^2}.$$

Since the entries of M^{-1} are given by $(-1)^{i+j}\det M_{ij}/\det M$, from the graph-theoretic explanation of the (i,j) minor $\det M_{ij}$ in Corollary 3.1.3, we see that (3.17) implies

$$\mathcal{G}(x,y) = \frac{1}{\mathrm{vol}(\Gamma)^2\tau(\Gamma)}\left(\sum_{P\in\mathscr{P}_\Gamma(x,y)}\Big(R(\Gamma-P;d_\Gamma)+Z(\Gamma-P;d_\Gamma)\Big)\right.$$
$$\left.-\sum_{\substack{u,v\in V(\Gamma)\\ u\neq v}}\ \sum_{\substack{P_1\in\mathscr{P}_\Gamma(x,u)\\ P_2\in\mathscr{P}_\Gamma(y,v)\\ P_1\cap P_2=\emptyset}} d_u d_v R(\Gamma-\{P_1,P_2\};d_\Gamma)\right) - \frac{1}{\mathrm{vol}(\Gamma)^2}.$$

Apply the second equation in Lemma 3.1.13

$$\sum_{P\in\mathscr{P}_\Gamma(x,y)} R(\Gamma-P;d_\Gamma) = \tau(\Gamma),$$

we arrive at (3.15).

Finally for the on-diagonal discrete Green's function, applying $R(\Gamma-\{x\};d_\Gamma)=\tau(\Gamma)$ to (3.15), we get

$$\begin{aligned}\mathcal{G}(x,x) &= \frac{1}{\mathrm{vol}(\Gamma)^2\tau(\Gamma)}\Big(R(\Gamma-\{x\};d_\Gamma)+Z(\Gamma-\{x\};d_\Gamma)\Big) - \frac{1}{\mathrm{vol}(\Gamma)^2}\\ &= \frac{Z(\Gamma-\{x\};d_\Gamma)}{\mathrm{vol}(\Gamma)^2\tau(\Gamma)}\end{aligned}$$

as claimed. □

Corollary 3.1.15. *We have $R(\Gamma;d_\Gamma)=0$ and if Γ is connected, we have*

$$Z(\Gamma;d_\Gamma) = \mathrm{vol}(\Gamma)^2\tau(\Gamma). \tag{3.20}$$

Proof. $R(\Gamma; d_\Gamma)$ is equal to the determinant of the Laplacian L of Γ, so $R(\Gamma; d_\Gamma) = 0$ follows from Lemma 3.1.11.

For the M_s defined in (3.18), we have

$$\begin{aligned} M_s &= D^{-1/2}(\mathcal{L} + D^{1/2} s J D^{1/2}) D^{-1/2} \\ &= D^{-1/2} \Phi \operatorname{diag}[\operatorname{vol}(\Gamma) s, \lambda_2, \ldots, \lambda_n] \Phi^t D^{-1/2}, \end{aligned}$$

so its determinant equals

$$\det M_s = \frac{\operatorname{vol}(\Gamma)^2 \tau(\Gamma) \cdot s}{(\prod_{x \in V(\Gamma)} d_x)^2}. \tag{3.21}$$

Then the corollary follows from (3.19). □

3.2 GREEN'S FUNCTIONS OF SOME SPECIAL GRAPHS

We will use a sequence $w = [w_1, \ldots, w_n]$ to denote the weight function of a labeled vertex-weighted graph (with vertices labeled $1, \ldots, n$). In most cases, this will not cause confusion. The method of proof is to apply the recursive formulas (3.9), (3.10) and the initial values (3.4) to get explicit formulas of Chung-Yau invariants for some special vertex-weighted graphs. They are useful in the calculation of discrete Green's functions and hitting times.

Lemma 3.2.1. *For a path on n vertices P_n with weight $w = [2, \ldots, 2] = [2^n]$,*

$$R(P_n; 2^n) = n + 1, \tag{3.22}$$

$$Z(P_n; 2^n) = \frac{1}{3} n(n+1)^2(n+2). \tag{3.23}$$

Proof. Let $r_n = R(P_n; 2^n)$. Let x be the leftmost vertex of P_n. By (3.9) we have

$$r_n = 2r_{n-1} - r_{n-2}$$

Since $r_0 = 1, r_1 = 2$, we get $r_n = n + 1$.

Let $z_n = Z(P_n; 2^n)$. By (3.10), we have

$$z_n = 2z_{n-1} - z_{n-2} + 4n + 8 \sum_{i=0}^{n-2} (i+1)$$

$$= 2z_{n-1} - z_{n-2} + 4n^2.$$

Since $z_0 = 0, z_1 = 4$, it is not difficult check that $z_n = \frac{1}{3}n(n+1)^2(n+2)$ satisfy the above recursion formula. Hence it is the unique solution. □

The proofs of the following lemmas are similar and thus omitted.

Lemma 3.2.2. *Let* $w = [1, 2, \ldots, 2] = [1, 2^{n-1}]$. *Then*

$$R(P_n; [1, 2^{n-1}]) = 1,$$

$$Z(P_n; [1, 2^{n-1}]) = \frac{4}{3}n^3 - \frac{1}{3}n.$$

Here the leftmost vertex of P_n *is assigned weight* 1.

Lemma 3.2.3. *Let* K_n, $n \geq 1$ *be the complete graph on* n *vertices. Then for any* m, *we have*

$$R(K_n; m^n) = (m - n + 1)(m + 1)^{n-1}, \tag{3.24}$$

$$Z(K_n; m^n) = n \cdot m^2(m + 1)^{n-1}. \tag{3.25}$$

Lemma 3.2.4. *Let* S_n, $n \geq 1$ *be the* n*-star graph with weight vector* $[m, 1^{n-1}]$ *that assigns* m *to the center vertex and* 1 *to* $n - 1$ *leaves. Then*

$$R(S_n; [m, 1^{n-1}]) = m - n + 1,$$

$$Z(S_n; [m, 1^{n-1}]) = m^2 - 3m + 3mn.$$

We will show that Theorem 3.1.14 is effective in obtaining closed formulas of discrete Green's functions, hence the hitting time of random walk via Theorem 3.0.1. We need the explicit formulas of $R(\Gamma; w)$ and $Z(\Gamma; w)$ derived in the previous lemmas.

Example 3.2.5. *We compute discrete Green's function of C_n, the cycle on $n \geq 3$ vertices. Let P_n denote the path on $n \geq 1$ vertices. First we have*

$$\mathcal{G}(x,x) = \frac{Z(P_{n-1}; 2^{n-1})}{(2n)^2 \cdot n} = \frac{(n+1)(n-1)}{12n}.$$

Since $\mathcal{G}(x,y)$ depends only on $|x-y|$, we may assume $x = 0$, $y = j$.

For brevity, we denote by A and B the two sums on the right-hand side of (3.15) respectively,

$$\begin{aligned} A &:= \sum_{P \in \mathscr{P}_{C_n}(x,y)} Z(C_n - P; d_{C_n}), \\ B &:= \sum_{\substack{u,v \in V(C_n) \\ u \neq v}} \sum_{\substack{P_1 \in \mathscr{P}_{C_n}(x,u) \\ P_2 \in \mathscr{P}_{C_n}(y,v) \\ P_1 \cap P_2 = \emptyset}} d_u d_v R(C_n - \{P_1, P_2\}; d_{C_n}). \end{aligned}$$

Then we apply the previous lemmas.

$$\begin{aligned} A &:= Z(P_{n-j-1}; 2^{n-j-1}) + Z(P_{j-1}; 2^{j-1}) \\ &= \frac{1}{3}\big(j^4 + (n-j)^4\big) - \frac{1}{3}\big(j^2 + (n-j)^2\big). \end{aligned}$$

and

$$\begin{aligned} B &:= 4\Bigg(j(n-j) + (n-j)\sum_{i=1}^{j-1} i(j-i+1) + j\sum_{i=1}^{n-j-1} i(n-j-i+1) \\ &\quad + \sum_{k=j+1}^{n-1}\sum_{\ell=1}^{j-1}\big((k-j)\ell + (n-k)(j-\ell)\big)\Bigg) \\ &= \frac{2}{3} j(j-n)(j^2 - nj - 1 - n^2). \end{aligned}$$

We get discrete Green's function of C_n,

$$\begin{aligned} \mathcal{G}(x,y) &= \frac{1}{(2n)^2 \cdot n}(A - B) \\ &= \frac{(n+1)(n-1)}{12n} - \frac{j(n-j)}{2n} \\ &= \frac{(n+1)(n-1)}{12n} - \frac{|x-y|(n-|x-y|)}{2n}. \end{aligned}$$

Example 3.2.6. *The discrete Green's function of P_n (with more general weights), has been computed by Chung and Yau [8]. From Lemma 3.2.2, for any $1 \leq x \leq y \leq n$, we get the Green's function of P_n,*

$$\mathcal{G}(x,y) = \frac{1}{12(n-1)}\big(6(x-1)^2 + 6(n-y)^2 - 2n^2 + 4n - 3\big).$$

Example 3.2.7. *For the complete graph K_n on n vertices, we have $\mathrm{vol}(K_n) = n(n-1)$ and $\tau(K_n) = n^{n-2}$. Discrete Green's function of K_n are given by*

$$\mathcal{G}(x,y) = \begin{cases} -\frac{1}{n^2} & \text{if } x \neq y, \\ \frac{n-1}{n^2} & \text{if } x = y. \end{cases}$$

Example 3.2.8. *Let c be the center of the star S_n and x, y distinct leaves of S_n. Then its discrete Green's functions are given by*

$$\mathcal{G}(c,c) = \frac{1}{4(n-1)}, \qquad \mathcal{G}(x,x) = \frac{4n-7}{4(n-1)},$$
$$\mathcal{G}(c,x) = \frac{-1}{4(n-1)}, \qquad \mathcal{G}(x,y) = \frac{-3}{4(n-1)}.$$

3.3 THE HITTING TIME OF RANDOM WALKS

By Theorem 3.0.1, Theorem 3.1.14 and Lemma 3.1.13, we immediately get the following explicit formula for the hitting time of random walks.

Theorem 3.3.1. *Let G be a connected graph and $x, y \in V(G)$. Then*

$$H(x,y) = \frac{1}{\mathrm{vol}(G)\tau(G)}\Bigg(Z(G-\{y\};d_G) - \sum_{P \in \mathscr{P}_G(x,y)} Z(G-P;d_G) + \sum_{\substack{u,v \in V(G) \\ u \neq v}} \sum_{\substack{P_1 \in \mathscr{P}_G(x,u) \\ P_2 \in \mathscr{P}_G(y,v) \\ P_1 \cap P_2 = \emptyset}} d_u d_v R(G - \{P_1, P_2\}; d_G)\Bigg). \quad (3.26)$$

Corollary 3.3.2. *Under the above notation, we have*

$$H(x,y) - H(y,x) = \frac{1}{\mathrm{vol}(G)\tau(G)}\Big(Z(G-\{y\};d_G) - Z(G-\{x\};d_G)\Big).$$

The above corollary gives a useful criterion to study reversible graphs (i.e., graphs with symmetric hitting times) in Chapter 5.

Corollary 3.3.3. *Let G be a connected graph and $x, y \in V(G)$. Then*

$$H(x,y) = \frac{1}{\mathrm{vol}(G)\tau(G)} \sum_{u,v\in V(G)} d_u d_v \left(\sum_{\substack{P\in\mathscr{P}_G(u,v)\\ y\notin P}} \tau(G/\{P,y\}) \right.$$

$$\left. - \sum_{\substack{P_1\in\mathscr{P}_G(x,y)\\ P_2\in\mathscr{P}_G(u,v)\\ P_1\cap P_2=\emptyset}} \tau(G/\{P_1,P_2\}) + \sum_{\substack{P_1\in\mathscr{P}_G(x,u)\\ P_2\in\mathscr{P}_G(y,v)\\ P_1\cap P_2=\emptyset}} \tau(G/\{P_1,P_2\}) \right), \quad (3.27)$$

where $G/\{P,y\}$ denotes the graph obtained by contracting P and y to a point and similarly for $G/\{P_1,P_2\}$. Note that $G/\{P,y\}$ and $G/\{P_1,P_2\}$ may be multigraphs.

Proof. Note that for any induced subgraph S of G, we have $R(\Gamma - \{S\}; d_\Gamma) = R(\Gamma/S)$ where Γ/S is the graph obtained from Γ by contracting S to a vertex. Then (3.27) follows readily from (3.26) and Lemma 3.1.10. □

The following formula is the main result we will apply in the remaining chapters of the thesis. We give a proof that is more intuitive than the original one.

Theorem 3.3.4 ([25, Theorem 2.7])**.** *For a connected graph G and $x, y \in V(G)$,*

$$H(x,y) = \frac{1}{\tau(G)} \sum_{u\in V(G)} d_u \sum_{\substack{P\in\mathscr{P}_G(x,u)\\ y\notin P}} \tau(G/\{P,y\}). \quad (3.28)$$

Here $\mathscr{P}_G(x,u)$ denotes the set of all simple paths (with no repeated vertices) connecting x and u in G. By convention $\mathscr{P}_G(x,x)$ consists of the trivial path $\{x\}$ only. For any subgraph S of G, we denote by $G/\{S\}$ the graph obtained from G by contracting S to a vertex.

Proof. We denote the bracket term of (3.27) by $F(x, y, u, v)$. The proof in [25] shows that for any fixed vertices x, y, u, $F(x, y, u, v)$ is independent of v. Then set $v = x$ in (3.27) gives the desired identity. Here we give a more intuitive proof of $F(x, y, u, v) = F(x, y, u, x)$.

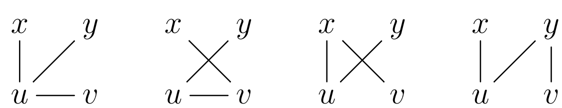
We modify G by adding an edge uy if u, y are not adjacent, namely we define a simple graph G' by

$$G' = \begin{cases} G & \text{if } u \sim y, \\ G \cup \{uy\} & \text{otherwise.} \end{cases} \tag{3.29}$$

Note that the following sum

$$\sum_{\substack{P \in \mathscr{P}_G(u,x) \\ y \notin P}} \tau(G/\{P, y\})$$

counts the number of spanning trees of G' which contains the edge uy and a path from u to x not containing y. They could be graphically described as the following four kinds of spanning trees of G'.

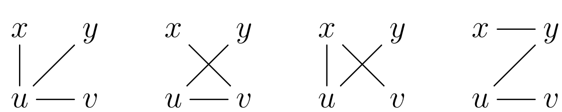


Here the line between u and y denotes the edge uy and all other lines denote simple paths.

Similarly the following sum

$$\sum_{\substack{P \in \mathscr{P}_G(u,v) \\ y \notin P}} \tau(G/\{P, y\})$$

counts the number of spanning trees of G' which contains the edge uy and a path from u to v not containing y. They could be graphically described as the following four kinds of spanning trees of G'.



Comparing the two groups of spanning trees, the first three terms are exactly the same trees. Hence

$$\sum_{\substack{P \in \mathscr{P}_G(u,x) \\ y \notin P}} \tau(G/\{P, y\}) - \sum_{\substack{P \in \mathscr{P}_G(u,v) \\ y \notin P}} \tau(G/\{P, y\})$$

$$
= \left[\begin{array}{ccc} x & & y \\ | & \diagup & | \\ u & & v \end{array} \right] - \left[\begin{array}{ccc} x & — & y \\ & \diagup & \\ u & — & v \end{array} \right]
$$

$$
= \sum_{\substack{P_1 \in \mathscr{P}_G(x,u) \\ P_2 \in \mathscr{P}_G(y,v) \\ P_1 \cap P_2 = \emptyset}} \tau(G/\{P_1, P_2\}) - \sum_{\substack{P_1 \in \mathscr{P}_G(x,y) \\ P_2 \in \mathscr{P}_G(u,v) \\ P_1 \cap P_2 = \emptyset}} \tau(G/\{P_1, P_2\}).
$$

We get (3.28) immediately from (3.27). □

In fact, Theorem 3.3.1 and 3.3.4 lead to more intuitive or direct proofs of most existing results on hitting times.

As an example, we give a proof of the following well-known result on the expected return time, i.e., the expected number of steps for a walker to return to the starting vertex after leaving it. The proof in [24] used Theorem 3.3.1. Here we give a simpler proof using Theorem 3.3.4.

Theorem 3.3.5. *Let G be a connected graph. Then the expected return time to a vertex $x \in V(G)$ is equal to*

$$
1 + \frac{1}{d_x} \sum_{\substack{y \in V(G) \\ y \sim x}} H(y, x) = \frac{\mathrm{vol}(G)}{d_x}.
$$

Proof. By (3.28), we have

$$
\begin{aligned}
\sum_{\substack{y \in V(G) \\ y \sim x}} H(y, x) &= \frac{1}{\tau(G)} \sum_{\substack{y \in V(G) \\ y \sim x}} \sum_{u \in V(G)} d_u \sum_{\substack{P \in \mathscr{P}_G(y,u) \\ x \notin P}} \tau(G/\{P, x\}) \\
&= \frac{1}{\tau(G)} \sum_{\substack{u \in V(G) \\ u \neq x}} d_u \sum_{P \in \mathscr{P}_G(x,u)} \tau(G/\{P\}) \\
&= \frac{1}{\tau(G)} \sum_{\substack{u \in V(G) \\ u \neq x}} d_u \tau(G) \\
&= \mathrm{vol}(G) - d_x,
\end{aligned}
$$

as claimed. □

Next we will prove an explicit formula for the hitting times of random walks on a tree T by applying (3.28). The enumeration of paths on a tree are relatively simple. For any two vertices $a, b \in V(T)$, there is a unique path $P_{a\to b}$ between a and b, whose length is the distance $d(a, b)$ between a and b.

The following explicit formula for the hitting time on trees was first obtained by Chen and Zhang [6] using the method of electric networks.

Theorem 3.3.6. *Let T be a tree and $a, b \in V(T)$ with $P_{a\to b}$ the unique path connecting a to b. For any $u \in V(P_{a\to b})$, we denote by T_u the component of $T - E(P_{a\to b})$ that contains u. Then the hitting time $H(a, b)$ satisfies*

$$H(a,b) = d(a,b)^2 + 2\sum_{u\in V(P_{a\to b})} |E(T_u)|d(u,b). \tag{3.30}$$

Proof. By (3.28), we have

$$\begin{aligned}
H(a,b) &= \frac{1}{\tau(T)}\left(\sum_{\substack{u\in V(P_{a\to b})\\ u\neq b}}\left(\sum_{x\in T_u} d_x\right)\tau(T/\{P_{a\to x}, b\})\right)\\
&= \sum_{u\in V(P_{a\to b})} d(u,b)\left(\sum_{x\in T_u} d_x\right)\\
&= 2\sum_{u\in V(P_{a\to b})} |E(T_u)|d(u,b) + d(a,b) + \sum_{i=1}^{d(a,b)-1} 2i\\
&= d(a,b)^2 + 2\sum_{u\in V(P_{a\to b})} |E(T_u)|d(u,b),
\end{aligned}$$

as claimed. □

As another application of (3.28), we give a proof of a formula of commute times in terms of the number of spanning trees, which was previously proved using the "topological formulas" from the electric networks (cf. [16]).

The proof of the following lemma can be found in [3].

Lemma 3.3.7. *For any $u \neq v \in V(G)$ and $x \in V(G)$,*

$$\sum_{\substack{P\in\mathscr{P}_G(x,u)\\ v\notin P}} \tau(G/\{P,v\}) + \sum_{\substack{P\in\mathscr{P}_G(x,v)\\ u\notin P}} \tau(G/\{P,u\}) = \tau(G/\{u,v\}).$$

Theorem 3.3.8. *Let $x, y \in V(G)$ be two distinct vertices and G' be the graph obtained from G by identifying x and y. Then we have*

$$H(x,y) + H(y,x) = \mathrm{vol}(G)\frac{\tau(G')}{\tau(G)}.$$

Proof. By (3.28), we have

$$\begin{aligned} H(x,y) + H(y,x) &= \frac{1}{\tau(G)} \sum_{u \in V(G)} d_u \left(\sum_{\substack{P \in \mathscr{P}_G(x,u) \\ y \notin P}} \tau(G/\{P,y\}) + \sum_{\substack{P \in \mathscr{P}_G(y,u) \\ x \notin P}} \tau(G/\{P,x\}) \right) \\ &= \frac{1}{\tau(G)} \sum_{u \in V(G)} d_u \tau(G/\{x,y\}) \\ &= \frac{1}{\tau(G)} \mathrm{vol}(G) \tau(G'). \end{aligned}$$

The 2nd equation used the above lemma. □

4.0 HITTING TIMES FOR GENERALIZED SUBDIVISION AND TRIANGULATION GRAPHS

The main work of the chapter is based on the formula (3.28) which expresses hitting times in terms of enumerations of paths and spanning trees.

Let G be a connected graph. For any positive integer $k \geq 1$, the k-th subdivision graph of G, denoted by $S_k(G)$, is the graph obtained by inserting k new vertices of degree 2 to each edge of G. Denoted by $Q_k(G)$ the graph obtained by adding a path of length k between any two adjacent vertices of G. We prove a formula expressing hitting times of $S_k(G)$ (res. $Q_k(G)$) in terms of those of G. Similar formulas were also proved for the degree-Kirchhoff index and electric resistance. It generalized the work of Chen [5] (for $k = 1$) and Huang-Li [12] (for $k = 2$), but with different method.

4.1 HITTING TIMES OF RANDOM WALKS ON $S_K(G)$

Let G be a graph with n vertices and m edges. For any positive integer $k \geq 1$, the k-th subdivision graph of G, denoted by $S_k(G)$, is the graph obtained by inserting k new vertices of degree 2 to each edge of G. Then $S_k(G)$ has $n + km$ vertices and $(k+1)m$ edges. Denote $V(S_k(G)) = V \cup V'$, where V is the set of original vertices in G, and V' is the set of newly inserted vertices.

If $i \in V'$ is inserted on the edge $st \in E(G)$, we will denote $\Gamma(i) = (s, t)$ and also regard i an integer $1 \leq i \leq k$ with $s = 0$ and $t = k + 1$. In fact, for $i \in V$ incident to an edge $st \in E(G)$, we also denote $\Gamma(i) = (s, t)$, we may regard $i = 0$ if $i = s$ and $i = k + 1$ if $i = t$.

The above notations will be used in the following lemmas and theorems.

Lemma 4.1.1. *For any multigraph G with n vertices and m edges, we have*

$$\tau(S_k(G)) = (k+1)^{m-n+1}\tau(G).$$

Proof. To obtain a spanning tree of G, we need to remove exactly $m-n+1$ edges from G. Since $S_k(G)$ is obtained by replacing each edge e of G by a path P_e of length $k+1$, removing an edge e from G corresponds to removing one of the $k+1$ edges from P_e in $S_k(G)$. The assertion follows easily. □

Lemma 4.1.2. *Let P be any simple path of G and $j \notin P$ a vertex of G not on P. We may also naturally regard P as a path in $S_k(G)$. Then*

$$\tau(S_k(G)/\{P,j\}) = (k+1)^{m-n+2}\tau(G/\{P,j\}).$$

Proof. If P has length l, then $G/\{P,j\}$ is a graph with $n-l-1$ vertices and $m-l$ edges. Note that $S_k(G)/\{P,j\} = S_k(G/\{P,j\})$, so the assertion follows from Lemma 4.1.1. □

Theorem 4.1.3. *If $i,j \in V$, then $H_{S_k(G)}(i,j) = (k+1)^2 H_G(i,j)$.*

Proof. Apply (3.28) and split the calculation into two terms

$$\begin{aligned} H_{S_k(G)}(i,j) &= \frac{1}{\tau(S_k(G))}\left(\sum_{u\in V} d_u \sum_{\substack{P\in\mathscr{P}_{S_k(G)}(i,u)\\ j\notin P}} \tau(S_k(G)/\{P,j\}) \right.\\ &\qquad\left. + \sum_{u\in V'} 2 \sum_{\substack{P\in\mathscr{P}_{S_k(G)}(i,u)\\ j\notin P}} \tau(S_k(G)/\{P,j\})\right)\\ &= A + B. \end{aligned}$$

By Lemma 4.1.1 and 4.1.2, we have

$$\begin{aligned} A &= \frac{1}{\tau(S_k(G))}\sum_{u\in V} d_u \sum_{\substack{P\in\mathscr{P}_{S_k(G)}(i,u)\\ j\notin P}} \tau(S_k(G)/\{P,j\})\\ &= \frac{1}{(k+1)^{m-n+1}\tau(G)}\sum_{u\in V} d_u \sum_{\substack{P\in\mathscr{P}_{G}(i,u)\\ j\notin P}} (k+1)^{m-n+2}\tau(G/\{P,j\}) \end{aligned}$$

$$= (k+1)H_G(i,j).$$

For the calculation of B, we introduce some notations. Let $e \in E(G)$ be an edge of G, we use $a_e, b_e \in V(G)$ to denote the two vertices incident to e and $u_t, 1 \le t \le k$ to denote the newly inserted vertices on e in $S_k(G)$.

$$B = \frac{1}{\tau(S_k(G))} \sum_{e \in E(G)} \sum_{t=1}^{k} 2 \left(\sum_{\substack{P \in \mathscr{P}_G(i,a_e) \\ e,j \notin P}} \tau(S_k(G)/\{P, j, \overline{a_e u_t}\}) + \sum_{\substack{P \in \mathscr{P}_G(i,b_e) \\ e,j \notin P}} \tau(S_k(G)/\{P, j, \overline{b_e u_t}\}) \right)$$

where $\overline{a_e u_t}$ (resp. $\overline{b_e u_t}$) denotes the path connecting a_e (resp. b_e) and u_t on e.

Look at the first term of the above bracket. Consider a path $P \in \mathscr{P}_G(i, a_e)$ with $e, j \notin P$. We separate the calculation of $\tau(S_k(G)/\{P, j, \overline{a_e u_t}\})$ into two cases.

(1) If $b_e = j$ or $b_e \in P$, then $\overline{u_t b_e}$ is a cycle of length $k+1-t$ in $S_k(G)/\{P, j, \overline{a_e u_t}\}$. Hence

$$\tau(S_k(G)/\{P, j, \overline{a_e u_t}\}) = (k+1-t)\tau(S_k(G)/\{P, j\} \backslash \overline{a_e b_e})$$

(2) If $b_e \ne j$ and $b_e \notin P$, then $\overline{u_t b_e}$ is not a cycle in $S_k(G)/\{P, j, \overline{a_e u_t}\}$. We divide the spanning trees of $S_k(G)/\{P, j, \overline{a_e u_t}\}$ into two groups depending on whether it contains $\overline{u_t b_e}$ or not. Hence

$$\tau(S_k(G)/\{P, j, \overline{a_e u_t}\}) = \tau(S_k(G)/\{P, j, \overline{a_e b_e}\}) + (k+1-t)\tau(S_k(G)/\{P, j\} \backslash \overline{a_e b_e})$$

It is not difficult to prove the following two identities

$$\sum_{\substack{P \in \mathscr{P}_G(i,a_e) \\ e,j \notin P \\ b_e \ne j, b_e \notin P}} \tau(G/\{P, j, e\}) = \sum_{\substack{P \in \mathscr{P}_G(i,b_e) \\ e \in P, j \notin P}} \tau(G/\{P, j\})$$

and

$$\sum_{\substack{P \in \mathscr{P}_G(i,a_e) \\ e,j \notin P \\ b_e \ne j, b_e \notin P}} \tau(G/\{P, j, e\}) + \sum_{\substack{P \in \mathscr{P}_G(i,a_e) \\ e,j \notin P}} \tau(G/\{P, j\} \backslash e) = \sum_{\substack{P \in \mathscr{P}_G(i,a_e) \\ e,j \notin P}} \tau(G/\{P, j\})$$

From the above two identities and Lemma 4.1.2, we have

$$\sum_{t=1}^{k} 2 \sum_{\substack{P \in \mathscr{P}_G(i,a_e) \\ e,j \notin P}} \tau(S_k(G)/\{P, j, \overline{a_e u_t}\})$$

$$
\begin{aligned}
=&\sum_{t=1}^{k} 2 \sum_{\substack{P\in\mathscr{P}_G(i,a_e)\\ e,j\notin P\\ b_e=j \text{ or } b_e\in P}} (k+1-t)\tau(S_k(G)/\{P,j\}\backslash\overline{a_eb_e})\\
&+\sum_{t=1}^{k} 2 \sum_{\substack{P\in\mathscr{P}_G(i,a_e)\\ e,j\notin P\\ b_e\neq j, b_e\notin P}} \Big(\tau(S_k(G)/\{P,j,\overline{a_eb_e}\}) + (k+1-t)\tau(S_k(G)/\{P,j\}\backslash\overline{a_eb_e})\Big)\\
=&\sum_{\substack{P\in\mathscr{P}_G(i,a_e)\\ e,j\notin P\\ b_e\neq j, b_e\notin P}} 2k(k+1)^{m-n+2}\tau(G/\{P,j,e\}) + \sum_{\substack{P\in\mathscr{P}_G(i,a_e)\\ e,j\notin P}} k(k+1)^{m-n+2}\tau(G/\{P,j\}\backslash e)\\
=&k(k+1)^{m-n+2}\left(\sum_{\substack{P\in\mathscr{P}_G(i,a_e)\\ e,j\notin P}}\tau(G/\{P,j\}) + \sum_{\substack{P\in\mathscr{P}_G(i,b_e)\\ e\in P, j\notin P}}\tau(G/\{P,j\})\right).
\end{aligned}
$$

Here $\cdots\backslash\overline{a_eb_e}$ denotes the graph which removes the path $\overline{a_eb_e}$ while keeping vertices a_e, b_e, and $\cdots\backslash e$ denotes the graph which removes the edge e while keeping vertices a_e, b_e. Similarly,

$$
\begin{aligned}
&\sum_{t=1}^{k} 2 \sum_{\substack{P\in\mathscr{P}_G(i,b_e)\\ e,j\notin P}} \tau(S_k(G)/\{P,j,\overline{b_eu_t}\})\\
=&k(k+1)^{m-n+2}\left(\sum_{\substack{P\in\mathscr{P}_G(i,b_e)\\ e,j\notin P}}\tau(G/\{P,j\}) + \sum_{\substack{P\in\mathscr{P}_G(i,a_e)\\ e\in P, j\notin P}}\tau(G/\{P,j\})\right).
\end{aligned}
$$

Adding up the previous two equations, we get

$$
\begin{aligned}
B=&\frac{1}{(k+1)^{m-n+1}\tau(G)}\sum_{e\in E(G)} k(k+1)^{m-n+2}\left(\sum_{\substack{P\in\mathscr{P}_G(i,a_e)\\ j\notin P}}\tau(G/\{P,j\}) + \sum_{\substack{P\in\mathscr{P}_G(i,b_e)\\ j\notin P}}\tau(G/\{P,j\})\right)\\
=&\frac{k(k+1)}{\tau(G)}\sum_{u\in V} d_u \sum_{\substack{P\in\mathscr{P}_G(i,u)\\ j\notin P}}\tau(G/\{P,j\})\\
=&k(k+1)H_G(i,j).
\end{aligned}
$$

Adding up A and B gives the desired identity. □

Theorem 4.1.4. *If $i\in V\cup V'$, $j\in V$, $\Gamma(i)=(s,t)$, then*

$$
H_{S_k(G)}(i,j) = (k+1)(k+1-i)H_G(s,j) + (k+1)iH_G(t,j) + i(k+1-i). \tag{4.1}
$$

Proof. Note that when we set $i = 0$ (namely $i = s$) in (4.1), we get

$$H_{S_k(G)}(0, j) = (k+1)^2 H_G(s, j). \tag{4.2}$$

When we set $i = k+1$ (namely $i = t$) in (4.1), we get

$$H_{S_k(G)}(k+1, j) = (k+1)^2 H_G(t, j). \tag{4.3}$$

These identities coincide with Theorem 4.1.3.

By the first step analysis, we need to verify that for any $1 \le i \le k$, the given formula (4.1) of $H_{S_k(G)}(i, j)$ satisfies the recursive formula

$$H_{S_k(G)}(i, j) = 1 + \frac{1}{2}\big(H_{S_k(G)}(i-1, j) + H_{S_k(G)}(i+1, j)\big), \tag{4.4}$$

which is easy to check.

Next we show that the solution to the system of questions (4.4) is unique.

Fix j and let $a_i = H_{S_k(G)}(i, j)$. The k equations in (4.4) are

$$\frac{1}{2}a_{i-1} - a_i + \frac{1}{2}a_{i+1} = -1. \tag{4.5}$$

The $n \times n$ coefficient matrix

$$\begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & & \ddots & \\ & & 1 & -2 \end{bmatrix}$$

is a tridiagonal matrix and has nonzero determinant

$$f_n = (-1)^n \frac{n+1}{2^n}.$$

Hence the uniqueness of the solution of (4.4) is proved.

In other words, we have checked that (4.1) is the unique solution of $H_{S_k(G)}(i, j)$ which satisfies (4.2), (4.3) and (4.4). □

Theorem 4.1.5. *If $i \in V$, $j \in V \cup V'$, $\Gamma(j) = (p, q)$, then*

$$\begin{aligned} H_{S_k(G)}(i,j) =& (k+1)(k+1-j)H_G(i,p) + (k+1)jH_G(i,q) \\ &+ j(k+1-j)(2m - H_G(p,q) - H_G(q,p)) - j(k+1-j). \end{aligned} \tag{4.6}$$

Proof. When $j \in V$ this is true by Theorem 4.1.3. We may assume $j \in V'$. Hence $1 \leq j \leq k$. Apply (3.28) and split the calculation into two terms

$$\begin{aligned} H_{S_k(G)}(i,j) &= \frac{1}{\tau(S_k(G))} \left(\sum_{u \in V} d_u \sum_{\substack{P \in \mathscr{P}_{S_k(G)}(i,u) \\ j \notin P}} \tau(S_k(G)/\{P, j\}) \right. \\ &\qquad \left. + \sum_{u \in V'} 2 \sum_{\substack{P \in \mathscr{P}_{S_k(G)}(i,u) \\ j \notin P}} \tau(S_k(G)/\{P, j\}) \right) \\ &= A + B. \end{aligned}$$

The remaining proof is similar to that of Theorem 4.1.3. $\square$

Theorem 4.1.6. *If $i \in V \cup V'$, $j \in V \cup V'$, $\Gamma(i) = (s,t)$, $\Gamma(j) = (p, q)$, then*

$$\begin{aligned} H_{S_k(G)}(i,j) =& (k+1-i)(k+1-j)H_G(s,p) + (k+1-i)jH_G(s,q) \\ &+ i(k+1-j)H_G(t,p) + ijH_G(t,q) + i(k+1-i) - j(k+1-j) \\ &+ j(k+1-j)(2m - H_G(p,q) - H_G(q,p)) - \varepsilon(k,i,j). \end{aligned} \tag{4.7}$$

Here $\varepsilon(k,i,j)$ is given by

$$\varepsilon(k,i,j) = \begin{cases} 0, & \text{if } i,j \text{ are on different edges of } G; \\ 2mi(k+1-j), & \text{if } i,j \text{ are on the same edge of } G \text{ and } i \leq j; \\ 2mj(k+1-i), & \text{if } i,j \text{ are on the same edge of } G \text{ and } i \geq j. \end{cases}$$

Proof. Firstly it is not difficult to check that when $i \in V$ (i.e. $i = 0$ or $k+1$), (4.7) reduces to (4.6).

Secondly we could check that the given $H_{S_k(G)}(i,j)$ in (4.7) satisfies the equation arising from the first step analysis. Namely for any $1 \le i \le k$, if i, j are on different edges of G,

$$H_{S_k(G)}(i,j) = 1 + \frac{1}{2}\big(H_{S_k(G)}(i-1,j) + H_{S_k(G)}(i+1,j)\big). \tag{4.8}$$

If i, j are on same edge of G,

$$H_{S_k(G)}(i,j) = \begin{cases} 0, & i = j; \\ 1 + \frac{1}{2}\big(H_{S_k(G)}(i-1,j) + H_{S_k(G)}(i+1,j)\big), & i \neq j, 1 \le i \le k. \end{cases} \tag{4.9}$$

Finally we show that the solution to either system of questions (4.8) or (4.9) is unique. The uniqueness of the solution of (4.8) is already proved in the previous theorem. For the uniqueness of the solution of (4.9), we have the $n \times n$ coefficient matrix

$$\begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & & \ddots & & & \\ & & 0 & -2 & 0 & \\ & & & & \ddots & \\ & & & & 1 & -2 \end{bmatrix}$$

Also, the determinant is not zero. Hence the uniqueness of the solution of (4.9) is proved.

□

Corollary 4.1.7. *If G is a tree with $i \in V \cup V'$, $j \in V \cup V'$, $\Gamma(i) = (s,t)$, $\Gamma(j) = (p,q)$, then*

$$\begin{aligned} H_{S_k(G)}(i,j) =& (k+1-i)(k+1-j)H_G(s,p) + (k+1-i)jH_G(s,q) \\ &+ i(k+1-j)H_G(t,p) + ijH_G(t,q) + i(k+1-i) - j(k+1-j) \\ &- \varepsilon(k,i,j). \end{aligned} \tag{4.10}$$

Proof. For the tree G,

$$H_G(p,q) + H_G(q,p) = 2mr_{pq} = 2md_T(p,q) = 2m.$$

Hence, it follows from Theorem 4.1.6. □

Remark 4.1.8. *The equation (4.10) still holds if pq is a cut edge of G.*

4.2 HITTING TIMES OF RANDOM WALKS ON $Q_K(G)$

Let G be a graph with n vertices and m edges. For any positive integer $k \geq 2$, denoted by $Q_k(G)$ the graph obtained by adding a path of length k between any two adjacent vertices of G. Then $Q_k(G)$ has $n + (k-1)m$ vertices and $(k+1)m$ edges. Denote $V(Q_k(G)) = V \cup V'$, where V is the set of original vertices in G, and V' is the set of vertices on the newly added paths.

If $i \in V'$ is on the path connecting $s, t \in V$, we will denote $\Gamma(i) = (s,t)$ and regard i as an integer $1 \leq i \leq k-1$ with $s = 0$ and $t = k$. For convenience, when $i \in V$ is incident to an edge $st \in E(G)$, we also denote $\Gamma(i) = (s,t)$, and take $i = 0$ if $i = s$ and $i = k$ if $i = t$.

The above notations will be used throughout the section.

Lemma 4.2.1. *For any multigraph G with n vertices and m edges, we have*

$$\tau(Q_k(G)) = (k+1)^{n-1}k^{m-n+1}\tau(G).$$

Proof. A spanning tree of G has exactly $n-1$ edges, namely we need to remove exactly $m-n+1$ edges to get a spanning tree of G. Note that $Q_k(G)$ is obtained by attaching to each edge e of G a path P_e of length k connecting the two vertices of e. Pick a spanning tree T of G, we may obtain a set $S(T)$ of $(k+1)^{n-1}k^{m-n+1}$ spanning trees of $Q_k(G)$ as follows: if $e \in E(T)$, then remove exactly one edge on the cycle formed by e and P_e; if $e \notin E(T)$, then remove e and exactly one edge on the path P_e. For different spanning trees T of G, we get pairwise disjoint sets $S(T)$ of spanning trees of $Q_k(G)$. Moreover, the construction exhausts all spanning trees of $Q_k(G)$. We get the desired identity. □

Lemma 4.2.2. *Let G be a graph with n vertices and m edges. Let P be any simple path of G with length l and $j \notin P$ a vertex of G not on P. Then*

$$\tau(Q_k(G)/\{P,j\}) = k^l(k+1)^{n-l-2}k^{m-n+2}\tau(G/\{P,j\}).$$

Proof. If P has length l, then $G/\{P,j\}$ is a graph with $n-l-1$ vertices and $m-l$ edges. P can also be naturally regarded as a path in $Q_k(G)$. Note that $Q_k(G)/\{P,j\}$ is equal to the graph $Q_k(G/\{P,j\})$ plus l cycles of length k, so the assertion follows from Lemma 4.2.1. □

Theorem 4.2.3. *If $i,j \in V$, then $H_{Q_k(G)}(i,j) = kH_G(i,j)$.*

Proof. Apply (3.28) and split the calculation into two terms

$$\begin{aligned} H_{Q_k(G)}(i,j) &= \frac{1}{\tau(Q_k(G))}\left(\sum_{u\in V} 2d_u \sum_{\substack{P\in\mathscr{P}_{Q_k(G)}(i,u)\\ j\notin P}} \tau(Q_k(G)/\{P,j\}) \right.\\ &\qquad\left. + \sum_{u\in V'} 2 \sum_{\substack{P\in\mathscr{P}_{Q_k(G)}(i,u)\\ j\notin P}} \tau(Q_k(G)/\{P,j\})\right)\\ &= A+B. \end{aligned}$$

By Lemma 4.2.1 and 4.2.2, we have

$$\begin{aligned} A &= \frac{1}{\tau(Q_k(G))}\sum_{u\in V} 2d_u \sum_{\substack{P\in\mathscr{P}_{Q_k(G)}(i,u)\\ j\notin P}} \tau(Q_k(G)/\{P,j\})\\ &= \frac{1}{(k+1)^{n-1}k^{m-n+1}\tau(G)}\sum_{u\in V} 2d_u \sum_{\substack{P\in\mathscr{P}_{G}(i,u)\\ j\notin P}} \left(\sum_{i=0}^{l(P)}\binom{l(P)}{i}k^i\right)\\ &\qquad \times (k+1)^{n-l(P)-2}k^{m-n+2}\tau(G/\{P,j\})\\ &= \frac{1}{(k+1)^{n-1}k^{m-n+1}\tau(G)}\sum_{u\in V} 2d_u \sum_{\substack{P\in\mathscr{P}_{G}(i,u)\\ j\notin P}} (k+1)^{n-2}k^{m-n+2}\tau(G/\{P,j\})\\ &= \frac{2k}{k+1}H_G(i,j). \end{aligned}$$

Here $l(P)$ is the length of P.

For the calculation of B, we introduce some notations. Let $e \in E(G)$ be an edge of G, we use $a_e, b_e \in V(G)$ to denote the two vertices incident to e and $u_t, 1 \le t \le k-1$ to denote the new vertices on the newly added path P_e in $Q_k(G)$.

$$B = \frac{1}{\tau(Q_k(G))} \sum_{e\in E(G)} \sum_{t=1}^{k-1} 2 \left(\sum_{\substack{P\in \mathscr{P}_G(i,a_e)\\ e,j\notin P}} \frac{(k+1)^{l(P)}}{k^{l(P)}} \tau(Q_k(G)/\{P, j, \overline{a_e u_t}\}) + \sum_{\substack{P\in \mathscr{P}_G(i,b_e)\\ e,j\notin P}} \frac{(k+1)^{l(P)}}{k^{l(P)}} \tau(Q_k(G)/\{P, j, \overline{b_e u_t}\}) \right),$$

where $\overline{a_e u_t}$ (resp. $\overline{b_e u_t}$) denotes the path connecting a_e (resp. b_e) and u_t on P_e. In the first term, the set of spanning trees of $Q_k(G)/\{P, j, \overline{a_e u_t}\}$ could be divided into two cases depending on whether the spanning tree contains $\overline{u_t b_e}$ or not. Hence

$$\begin{aligned}
&\sum_{t=1}^{k-1} 2 \sum_{\substack{P\in \mathscr{P}_G(i,a_e)\\ e,j\notin P}} \frac{(k+1)^{l(P)}}{k^{l(P)}} \tau(Q_k(G)/\{P, j, \overline{a_e u_t}\}) \\
=&\sum_{t=1}^{k-1} 2 \sum_{\substack{P\in \mathscr{P}_G(i,a_e)\\ e,j\notin P}} \frac{(k+1)^{l(P)}}{k^{l(P)}} \left(\tau(Q_k(G)/\{P, j, \overline{a_e b_e}\}) + (k-t)\tau(Q_k(G)/\{P, j\}\backslash \overline{a_e b_e}) \right) \\
=& \sum_{\substack{P\in \mathscr{P}_G(i,a_e)\\ e,j\notin P}} 2(k-1)(k+1)^{n-2} k^{m-n+2} \tau(G/\{P, j, e\}) \\
&\qquad + (k-1)(k+1)^{n-2} k^{m-n+2} \tau(G/\{P, j\}\backslash e) \\
=&(k-1)(k+1)^{n-2} k^{m-n+2} \left(\sum_{\substack{P\in \mathscr{P}_G(i,a_e)\\ e,j\notin P}} \tau(G/\{P, j\}) + \sum_{\substack{P\in \mathscr{P}_G(i,b_e)\\ e\in P, j\notin P}} \tau(G/\{P, j\}) \right).
\end{aligned}$$

Here $\cdots \backslash \overline{a_e b_e}$ denotes the graph which removes the path $\overline{a_e b_e}$ while keeping vertices a_e, b_e, and $\cdots \backslash e$ denotes the graph which removes the edge e while keeping vertices a_e, b_e. Similarly,

$$\begin{aligned}
&\sum_{t=1}^{k-1} 2 \sum_{\substack{P\in \mathscr{P}_G(i,b_e)\\ e,j\notin P}} \frac{(k+1)^{l(P)}}{k^{l(P)}} \tau(Q_k(G)/\{P, j, \overline{b_e u_t}\}) \\
=&(k-1)(k+1)^{n-2} k^{m-n+2} \left(\sum_{\substack{P\in \mathscr{P}_G(i,b_e)\\ e,j\notin P}} \tau(G/\{P, j\}) + \sum_{\substack{P\in \mathscr{P}_G(i,a_e)\\ e\in P, j\notin P}} \tau(G/\{P, j\}) \right).
\end{aligned}$$

Adding up the above two equations, we get

$$
\begin{aligned}
B =& \frac{1}{(k+1)^{n-1}k^{m-n+1}\tau(G)} \sum_{e\in E(G)} (k-1)(k+1)^{n-2}k^{m-n+2} \\
& \times \left(\sum_{\substack{P\in\mathscr{P}_G(i,a_e)\\ j\notin P}} \tau(G/\{P,j\}) + \sum_{\substack{P\in\mathscr{P}_G(i,b_e)\\ j\notin P}} \tau(G/\{P,j\}) \right) \\
=& \frac{k(k-1)}{(k+1)\tau(G)} \sum_{u\in V} d_u \sum_{\substack{P\in\mathscr{P}_G(i,u)\\ j\notin P}} \tau(G/\{P,j\}) \\
=& \frac{k(k-1)}{k+1} H_G(i,j).
\end{aligned}
$$

Adding up A and B gives the desired identity. □

Theorem 4.2.4. *If $i \in V \cup V'$, $j \in V$, $\Gamma(i) = (s,t)$, then*

$$H_{Q_k(G)}(i,j) = (k-i)H_G(s,j) + iH_G(t,j) + i(k-i). \tag{4.11}$$

Proof. Note that when we set $i = 0$ (namely $i = s$) in (4.11), we get

$$H_{Q_k(G)}(0,j) = kH_G(s,j). \tag{4.12}$$

When we set $i = k$ (namely $i = t$) in (4.11), we get

$$H_{Q_k(G)}(k+1,j) = kH_G(t,j). \tag{4.13}$$

These identities coincide with Theorem 4.2.3.

Similar to the proof of Theorem 4.1.4, we only need to verify the system of equations from the first step analysis. Namely for any $1 \le i \le k$, the given formula (4.11) of $H_{Q_k(G)}(i,j)$ satisfies the recursive formula

$$H_{Q_k(G)}(i,j) = 1 + \frac{1}{2}\big(H_{Q_k(G)}(i-1,j) + H_{Q_k(G)}(i+1,j)\big), \tag{4.14}$$

which is easy to check.

In other words, we have checked that (4.11) is the unique solution of $H_{Q_k(G)}(i,j)$ which satisfies (4.12), (4.13) and (4.14). □

We refer the readers to the paper [20] for the more complete treatment of hitting times on $Q_k(G)$.

4.3 SOME GRAPH INVARIANTS OF $S_K(G)$

If $i, j \in V$, it is easy to see that $r_{ij}(S_k(G)) = (k+1)r_{ij}(G)$. In general, we can derive from Theorem 4.1.6 the following formula of electric resistance between any two vertices of $S_k(G)$.

Theorem 4.3.1. *If $i \in V \cup V'$, $j \in V \cup V'$, $\Gamma(i) = (s,t)$, $\Gamma(j) = (p,q)$, then*

$$r_{ij}(S_k(G)) = \frac{(k+1-i)(k+1-j)r_{ps}(G) + j(k+1-i)r_{qs}(G) + i(k+1-j)r_{pt}(G)}{k+1} + \frac{j(k+1-j)(1-r_{pq}(G)) + i(k+1-i)(1-r_{st}(G)) + ijr_{tq}(G)}{k+1} - \delta(k,i,j) \tag{4.15}$$

Here $\delta(k,i,j)$ is given by

$$\delta(k,i,j) = \begin{cases} 0, & \text{if } i,j \text{ are on different edges of } G; \\ \frac{2i(k+1-j)}{k+1}, & \text{if } i,j \text{ are on the same edge of } G \text{ and } i \le j; \\ \frac{2j(k+1-i)}{k+1}, & \text{if } i,j \text{ are on the same edge of } G \text{ and } i \ge j. \end{cases}$$

Proof. The resistance is related to the hitting time by

$$r_{xy} = \frac{H(x,y) + H(y,x)}{2m}, \tag{4.16}$$

so it follows easily from Theorem 4.1.6. □

In particular, when $k = 1$ and $i, j \in V'$ are on different edges of G, the formula (4.15) becomes

$$r_{ij}(S(G)) = \frac{r_{ps} + r_{pt} + r_{qs} + r_{qt} - r_{pq} - r_{st}}{2} + 1, \tag{4.17}$$

which is just [5, Theorem 5.3 (v)].

Recall the following well-known formula.

Lemma 4.3.2. *For any graph with n vertices, we have*

$$\frac{1}{2m} \sum_{xy \in E(G)} (H(x,y) + H(y,x)) = n - 1. \tag{4.18}$$

Theorem 4.3.3. *We have*

$$Kf^*(S_k(G)) = (k+1)^3 Kf^*(G) + \frac{1}{6}k(k+1)(k+2)(4m^2 - 4mn + 2m). \tag{4.19}$$

Proof. Firstly, we divide the case into $y \in V$ and $y \in V'$, where we have

$$\begin{aligned}
&Kf^*(S_k(G)) \\
=&\sum_{y\in V} d_y H_{S_k(G)}(x,y) + \sum_{y\in V'} 2H_{S_k(G)}(x,y) \\
=&\sum_{y\in V} d_y (k+1)^2 H_G(x,y) + \sum_{pq\in E(G)} 2(k+1)\sum_{j=1}^{k} j(H_G(x,p)+H_G(x,q)) \\
&+ \sum_{pq\in E(G)} \sum_{j=1}^{k+1} j(k+1-j)2m - \sum_{pq\in E(G)} \sum_{j=1}^{k+1} j(k+1-j)(H_G(p,q)+H_G(q,p)) \\
&- \sum_{pq\in E(G)} \sum_{j=1}^{k+1} j(k+1-j) \\
=&(k+1)^2 Kf^*(G) + (k+1)^2 k \sum_{y\in V} d_y H_G(x,y) + \sum_{j=1}^{k+1} j(k+1-j)2m^2 \\
&- \sum_{j=1}^{k+1} j(k+1-j)(n-1)2m - \sum_{j=1}^{k+1} j(k+1-j)m \\
=&(k+1)^3 Kf^*(G) + \frac{1}{6}k(k+1)(k+2)(4m^2-4mn+2m),
\end{aligned}$$

as claimed. ∎

4.4 SOME EXAMPLES

Example 4.4.1. *Assume that a, b are two vertices on the cycle graph C_n with $1 \le a < b \le n$, and i, j belong to the edges $\{a, a+1\}$ and $\{b, b+1\}$ respectively, the hitting time of the k-th subdivision graph of C_n is*

$$H_{S_k(C_n)}(i,j) = \big((k+1)b + j - (k+1)a - i\big)\big((k+1)n - (k+1)b - j + (k+1)a + i\big),$$

where $0 \leq i, j \leq k+1$*. By applying Theorem 4.1.6, we also have*

$$\begin{aligned}
H_{S_k(C_n)}(i,j) =&(k+1-i)(k+1-j)(b-a)(n-b+a) + j(k+1-i)(b+1-a)(n-b-1+a) \\
&+ i(k+1-j)(b-a-1)(n-b+a+1) + ij(b-a)(n-b+a) \\
&+ i(k+1-i) + j(k+1-j) - \varepsilon(k,i,j) \\
=&\big((k+1)b + j - (k+1)a - i\big)\big((k+1)n - (k+1)b - j + (k+1)a + i\big).
\end{aligned}$$

Example 4.4.2. *Assume that* a, b *are two vertices on the cycle graph* C_n *with* $1 \leq a < b \leq n$*, and* i, j *belong to the edges* $\{a, a+1\}$ *and* $\{b, b+1\}$ *respectively, the resistance of the* k*-th subdivision graph of the cycle graph* C_n *is*

$$r_{ij}(S_k(C_n)) = \frac{\big((k+1)b + j - (k+1)a - i\big)\big(n(k+1) - (k+1)b - j + (k+1)a + i\big)}{n(k+1)},$$

where $0 \leq i, j \leq k+1$*. By applying Theorem 4.3.1, we also have*

$$\begin{aligned}
&r_{ij}(S_k(C_n)) \\
=& \frac{1}{n(k+1)}\Big((k+1-i)(k+1-j)(b-a)(n-b+a) + j(k+1-i)(b+1-a)(n-b-1+a) \\
&+ i(k+1-j)(b-a-1)(n-b+a+1) + i(k+1-i) + j(k+1-j) + ij(b-a)(n-b+a)\Big) \\
=& \frac{\big((k+1)b + j - (k+1)a - i\big)\big(n(k+1) - (k+1)b - j + (k+1)a + i\big)}{n(k+1)}.
\end{aligned}$$

Example 4.4.3. *The degree-Kirchhoff index of the* k*-th subdivision graph of the cycle graph* $S_k(C_n)$ *is*

$$\begin{aligned}
Kf^*(S_k(C_n)) &= 2\sum_{y=0}^{(k+1)n} y\big((k+1)n - y\big) \\
&= \frac{1}{3}(k+1)n(kn+n-1)(kn+n+1).
\end{aligned}$$

Since $Kf^*(C_n) = \frac{1}{3}(n-1)n(n+1)$*, by applying Theorem 4.3.3 to the cycle graph* C_n*, we also have*

$$\begin{aligned}
Kf^*(S_k(C_n)) &= (k+1)^3 Kf^*(C_n) + \frac{1}{3}k(k+1)(k+2)n \\
&= \frac{1}{3}(k+1)^3(n-1)n(n+1) + \frac{1}{3}k(k+1)(k+2)n \\
&= \frac{1}{3}(k+1)n(kn+n-1)(kn+n+1).
\end{aligned}$$

Example 4.4.4. *For a complete graph K_n, its degree-Kirchhoff index $Kf^*(K_n) = (n-1)^3$. By Theorem 4.3.3, the degree-Kirchhoff index of the subdivision graph $S_k(K_n)$ is equal to*

$$Kf^*(S_k(K_n)) = (k+1)^3(n-1)^3 + \frac{1}{6}kn(k+1)(k+2)(n-1)(n^2-3n+1). \tag{4.20}$$

5.0 CHUNG-YAU INVARIANTS AND REVERSIBLE GRAPHS

5.1 APPLICATIONS OF CHUNG-YAU INVARIANTS

Hitting times are related to many other interesting graph invariants. See [10, 13] for some recent works in this direction.

Below are two equations expressing discrete Green's function in terms of Chung-Yau invariants and hitting time.

Theorem 5.1.1. *For any $x \in V(G)$, we have*

$$\mathscr{G}(x,x) = \frac{d_x}{\mathrm{vol}(G)^2\tau(G)} Z(G - \{x\}) \tag{5.1}$$

and for any $x, y \in V(G)$,

$$\mathscr{G}(x,y) = \sqrt{d_x d_y}\left(\frac{Z(G-\{y\})}{\mathrm{vol}(G)^2\tau(G)} - \frac{H(x,y)}{\mathrm{vol}(G)}\right). \tag{5.2}$$

Proof. (5.1) is just (3.16). And (5.2) follows from Theorem 3.0.1 and (5.1). □

Recall the following closed formula (see (3.26) of Chapter 3) of hitting time in terms of Chung-Yau invariants.

Theorem 5.1.2 ([24, Theorem 4.1])**.** *For a connected graph G and $x, y \in V(G)$,*

$$H(x,y) = \frac{1}{\mathrm{vol}(G)\tau(G)}\Bigg(Z(G-\{y\}) - \sum_{P\in\mathscr{P}_G(x,y)} Z(G-\{P\}) + \sum_{\substack{u,v\in V(G)\\ u\neq v}} \sum_{\substack{P_1\in\mathscr{P}_G(x,u)\\ P_2\in\mathscr{P}_G(y,v)\\ P_1\cap P_2=\emptyset}} d_u d_v R(G-\{P_1,P_2\})\Bigg). \tag{5.3}$$

The formula (5.3) could be simplified to a closed formula (see (3.28) of Chapter 4) expressing the hitting time in terms of enumerations of paths and spanning trees.

Theorem 5.1.3 ([25, Theorem 2.7])**.** *For a connected graph G and $x, y \in V(G)$,*

$$H(x,y) = \frac{1}{\tau(G)} \sum_{u \in V(G)} d_u \sum_{\substack{P \in \mathscr{P}_G(x,u) \\ y \notin P}} \tau(G/\{P, y\}). \tag{5.4}$$

For a connected graph with n vertices and m edges, the *Kemeny's constant* $K(G)$ of G is defined by

$$K(G) = \frac{1}{\mathrm{vol}(G)} \sum_{y \in V(G)} d_y H(x,y), \tag{5.5}$$

which is known to be independent of $x \in V(G)$. Note that $\mathrm{vol}(G) = 2m$.

The *degree-Kirchhoff index* $Kf^*(G)$ is defined by (cf. [6])

$$Kf^*(G) = \frac{1}{2} \sum_{x,y \in V(G)} d_x d_y r_{xy}. \tag{5.6}$$

We have $Kf^*(G) = \mathrm{vol}(G)K(G)$ and $K(G) = \sum_{j=2}^{n} \frac{1}{\lambda_j}$, whose proofs can be found in [3, 10] and [16] respectively. We also have $K(G) = \sum_{x \in V(G)} \mathscr{G}(x,x)$ by the orthonormality of the eigenvectors $\{v_k\}$.

The formula (5.3) implies a formula of Kemeny's constant in terms of Chung-Yau invariants.

Proposition 5.1.4. *Let G be a connected graph. Then*

$$K(G) = \frac{1}{\mathrm{vol}(G)^2 \tau(G)} \sum_{x \in V(G)} d_x Z(G - \{x\}). \tag{5.7}$$

Proof. In (5.5), substitute $H(x,y)$ by the formula (5.3). Then in (5.3), substitute $Z(G - \{P\})$ by R-invariants using (3.12). It is not difficult to check that the second and third terms in the bracket of (5.3) exactly cancel. We get (5.7). □

The following proposition is a corollary of Theorem 5.1.3. As the proof in [3] is sketchy, here we give a detailed proof.

Proposition 5.1.5 ([3, Corollary 4.2]). *Let $d(x,y)$ be the graph distance of x, y on G. Then*

$$H(x,y) \le \sum_{\substack{u \in V(G) \\ u \neq y}} d_u \min\big(d(x,y), d(u,y)\big). \tag{5.8}$$

The equality holds when G is the path and x, y are the two end vertices.

Proof. Assume $x \neq y$, we construct a simple graph G_{xy} by

$$G_{xy} = \begin{cases} G & \text{if } x \sim y, \\ G \cup \{xy\} & \text{otherwise.} \end{cases}$$

Namely G_{xy} is obtained from G by adding an edge xy if x and y are not adjacent in G.

We use the notation $\Omega(G)$ to denote the set of spanning trees of G. It is not difficult to see that $\Omega(G/\{x,y\})$ is in one-to-one correspondence with the following subset of $\Omega(G_{xy})$.

$$\{T \in \Omega(G_{xy}) \mid T \text{ contains } xy\}.$$

Therefore we have

$$\tau(G/\{x,y\}) = \#\{T \in \Omega(G_{xy}) \mid T \text{ contains } xy\}. \tag{5.9}$$

For any $u \in V(G)$, define a subset S_u of $\Omega(G_{xy})$ by

$$S_u = \{T \in \Omega(G_{xy}) \mid T \text{ contains } xy \text{ and a path from } x \text{ to } u \text{ not passing through } y\}.$$

Then by (5.9) we have

$$\sum_{\substack{P \in \mathscr{P}_G(x,u) \\ y \notin P}} \tau(G/\{P,y\} = \#S_u \le \tau(G/\{x,y\}).$$

Similarly,

$$\sum_{\substack{P \in \mathscr{P}_G(x,u) \\ y \notin P}} \tau(G/\{P,y\} \le \tau(G/\{u,y\}).$$

By applying the above inequalities and $r_{xy} = \frac{\tau(G/\{x,y\})}{\tau(G)}$ to the formula (5.4), we get

$$H(x,y) = \frac{1}{\tau(G)} \sum_{\substack{u \in V(G) \\ u \neq y}} d_u \sum_{\substack{P \in \mathscr{P}_G(x,u) \\ y \notin P}} \tau(G/\{P,y\})$$

$$\leq \frac{1}{\tau(G)} \sum_{\substack{u\in V(G)\\ u\neq y}} d_u \min\Big(\tau(G/\{x,y\}), \tau(G/\{u,y\})\Big)$$

$$= \sum_{u\in V(G)} d_u \min(r_{xy}, r_{uy})$$

$$\leq \sum_{\substack{u\in V(G)\\ u\neq y}} d_u \min\big(d(x,y), d(u,y)\big),$$

where we used $r_{xy} \leq d(x,y)$ in the last inequality. □

The inequality (5.8) immediately implies the well-known upper bounded by $O(n^3)$ for hitting times. For a k-regular graph, we know (cf. [17]) that the diameter of G is upper bounded by $O(n/k)$. Hence by (5.8), we get the well-known fact that hitting times are upper bounded by $O(n^2)$ for regular graphs.

5.2 REVERSIBLE GRAPHS

As in [9], we call a connected graph G *reversible* if $H(x,y) = H(y,x)$ holds for any $x, y \in V(G)$.

Remark 5.2.1. *It is well-known that the following statements are equivalent:*

1. *G is reversible;*
2. *$\sum_{u\in V(G)} d_u R_{vu}$ is independent of the vertex v;*
3. *$\sum_{u\in V(G)} d_u H(u,v)$ is independent of the vertex v.*

The study of Chung-Yau invariants leads to an efficient criterion of checking whether a graph G is reversible.

Proposition 5.2.2 ([3])**.** *For any connected graph G and $x, y \in V(G)$,*

$$H(x,y) - H(y,x) = \frac{1}{\mathrm{vol}(G)\tau(G)}\left(\det B_{G-\{y\}} - \det B_{G-\{x\}}\right)\Big|_{s=1}, \tag{5.10}$$

where $B_{G-\{x\}}$ and $B_{G-\{y\}}$ are the matrices obtained from B in (3.6) by removing the row and column corresponding to the vertex x and y respectively.

In particular, G is reversible if and only if $\det B_{G-\{x\}}$ is independent of x.

Georgakopoulos [9] asked the following interesting questions: Is every reversible graph regular? If yes, is it even walk-regular?

Let A be the adjacency matrix of a connected G. Godsil and McKay [11] proved that a graph is walk-regular if and only if all order $n-1$ principal minors of $\lambda I - A$ are equal. On the other hand, if G is a d-regular graph, then Proposition 5.2.2 says that G is reversible if and only all order $n-1$ principal minors of $d^2 J + dI - A$ are equal, where J is an $n \times n$ matrix all of whose entries are equal to 1.

The following theorem was proved in [9]. A different proof was given in [3].

Theorem 5.2.3. *If G is a connected walk-regular graph, then G is reversible.*

For both of Georgakopoulos' questions, we are not able to find a counterexample. In [3], we gave some supporting evidence:[1]

(1) A reversible graph can have at most one cut edge. This is because if a graph G has a cut edge xy whose removal produces two connected subgraphs G_1 and G_2 where $x \in V(G_1)$ and $y \in V(G_2)$, then $H(x,y) = 2|E(G_1)| + 1$ and $H(y,x) = 2|E(G_2)| + 1$ (see [25, Rem. 2.11]).

(2) Vertex-transitive graphs are reversible. There is a cubic graph with 20 vertices which is walk-regular but not vertex-transitive [11].

(3) Let G_1, G_2 be two (not necessarily connected) vertex-transitive graphs, we can obtain a new graph G from the disjoint union graph $G_1 \cup G_2$ by adding an edge xy for each pair of vertices $x \in V(G_1)$, $y \in V(G_2)$. Note that the vertex set of G has at most two orbits under the action of $\mathrm{Aut}(G)$, so G is reversible if and only if $H(x,y) = H(y,x)$ for any fixed $x \in V(G_1)$, $y \in V(G_2)$. We have checked many cases of G_1 and G_2, but in all these cases, G is reversible if and only if G is walk-regular.

Now let us consider a special case of the above Item (3). Given a (not necessarily connected) vertex-transitive graph G, we can form a new augmented graph $\tilde{G}$ by adding a new vertex $\bullet$ which connects to each vertex of G. Note that when G is not a complete graph, the vertex set of $\tilde{G}$ has two orbits under the action of automorphisms of $\tilde{G}$.

Theorem 5.2.4 ([3])**.** *Let G be a vertex-transitive graph on n vertices. Then the augmented*

[1] We used graph data from the homepages of Gordon Royle and Brendan McKay.

graph $\tilde{G}$ is reversible if and only if G is a complete graph.

For random walks on a complete p-partite graph $K_{k_1,\dots,k_p}$, we know that $K_{k_1,\dots,k_p}$ is reversible if and only $k_1 = k_2 = \cdots = k_p$.

Definition 5.2.1. *A d-regular graph G is called almost walk-regular if for any integer $k \geq 1$, the diagonal elements of A^k differ by at most $d-2$.*

Recall the following linear algebra identity.

Lemma 5.2.5. *Let M be an $n \times n$ matrix and and u, v column vectors. Then*

$$\det(M + uv^T) = \det(M) + v^T \mathrm{adj}\,(M)u$$

Proof. Assume $M = I$, then

$$\det(M + uv^T) = \det(I + uv^T)$$

and

$$\det(M) + v^T \mathrm{adj}(M)u = 1 + v^T u$$

From

$$\begin{bmatrix} I & 0 \\ v^T & 1 \end{bmatrix} \begin{bmatrix} I + uv^T & u \\ 0 & 1 \end{bmatrix} \begin{bmatrix} I & 0 \\ -v^T & 1 \end{bmatrix} = \begin{bmatrix} I & u \\ 0 & 1 + v^T u \end{bmatrix},$$

we get $\det(I + uv^T) = 1 + v^T u$. While for general M,

$$\begin{aligned} \det(M + uv^T) &= \det(M(I + (M^{-1}u)v^T)) \\ &= \det(M)\det(I + (M^{-1}u)v^T) \\ &= \det(M)(1 + v^T M{-}1u) \\ &= \det(M) + v^T \mathrm{adj}(M)u, \end{aligned}$$

as claimed. □

In the rest of the section, we restrict to the case that G is a d-regular graph.

Proposition 5.2.6. *Let A be the adjacency matrix of a d-regular graph G. Then*

$$\det(d^2 J + dI - A) = \tau(G) n^2 d^2.$$

In particular, $d^2 J + dI - A$ is invertible.

Proof. In Lemma 5.2.5, take $M = dI - A$ and $u = v = (d, \dots, d)^T$. Then apply Lemma 3.1.11 and 3.1.12. Also note that $\det(dI - A) = 0$. □

Below is a very partial answer to Georgakopoulos' question.

Theorem 5.2.7. *If a d-regular graph G is reversible and almost walk-regular, then G is walk-regular.*

Proof. Since G is reversible, the diagonal elements of $(d^2 J + dI - A)^{-1}$ are equal. When $|x|$ is small,

$$\left(I + \left(dJ - \frac{A}{d}\right) x\right)^{-1} = I + \sum_{k=1}^{\infty} \left(dJ - \frac{A}{d}\right)^k x^k.$$

Let $f_i(x)$ be the i-th diagonal element of the left-hand side. Then we will see that $f_i(x) - f_j(x)$ has Taylor expansion with radius of convergence larger than 1 (since $d \geq 2$).

Let $a_k(i)$ be the i-th diagonal element of A^k. Note $AJ = JA = dJ$ and $J^2 = nJ$. Since G is reversible and almost walk-regular, for any $k \geq 1$ and $1 \leq i, j \leq n$ we have

$$\sum_{k=1}^{\infty} \frac{a_k(i) - a_k(j)}{d^k} = 0,$$

which implies that $a_k(i) = a_k(j)$, hence G is walk-regular. □

One may ask many questions about reversible graphs, such as: Whether a regular reversible graph is walk-regular (namely removing the almost regular condition in the above theorem). How to construct reversible graphs? Whether the cartesian product of two reversible graphs is still reversible. The last question is wide open as we even don't know whether the cartesian product of a reversible graph and the two-point path is always reversible or not.

The formula (5.4) is very useful in finding explicit formula of hitting times for special graphs.

Example 5.3.1. *We calculate hitting time of the cycle C_n. Let $1 \leq i < j \leq n$.*

For $1 \leq u \leq n$, we compute the contribution to the right-hand side of

$$\tau(C_n)H(i,j) = \sum_{u \in V(C_n)} d_u \sum_{\substack{P \in \mathscr{P}_{C_n}(x,u) \\ y \notin P}} \tau(C_n/\{P, y\}).$$

When $1 \leq u \leq i$, the contribution to $\tau(C_n)H(i,j)$ is

$$2\sum_{u=1}^{i}(j-i)(n-j+u) = i(j-i)(i-2j+2n+1).$$

When $i+1 \leq u \leq j-1$, the contribution to $\tau(C_n)H(i,j)$ is

$$2\sum_{u=i+1}^{j-1}(j-u)(n-j+i) = (j-i)(j-i-1)(n-j+i).$$

When $j+1 \leq u \leq n$, the contribution to $\tau(C_n)H(i,j)$ is

$$2\sum_{u=j+1}^{n}(j-i)(u-j) = (j-i)(n-j)(n-j+i).$$

Add up the above three terms and note that $\tau(C_n) = n$, we get $H(i,j) = (j-i)(n-j+i)$.

Example 5.3.2. *We calculate hitting time of the path P_n. Let $0 \leq i < j \leq n-1$.*

When $0 \leq u \leq i$, the contribution to $H(i,j)$ is

$$j - i + \sum_{u=1}^{i} 2(j-i) = (j-i)(2i+1).$$

When $i < u < j$, the contribution to $H(i,j)$ is

$$\sum_{u=i+1}^{j-1} 2(j-u) = (j-i)(j-i-1).$$

Hence $H(i,j) = (j-i)(2i+1) + (j-i)(j-i-1) = (j-i)(j+i)$.

Example 5.3.3. *We calculate hitting time of the complete graph K_n. By the result of [24, Lemma 3.3], we have that for any complete subgraph K_p of K_n,*

$$R(K_p) = (n-p)n^{p-1}.$$

An equivalent formulation is as follows: denote by $K_n(s)$ be the graph obtained from K_n by merging s vertices into a single vertex. Then its number of spanning trees $\tau(K_n(s)) = s \cdot n^{n-s-1}$.

Since $\tau(K_n) = n^{n-2}$, we have

$$\begin{aligned} H(x,y) &= \frac{1}{n^{n-2}} \sum_{k=0}^{n-2} (n-1) \binom{n-2}{k} k!(k+2) n^{n-3-k} \\ &= (n-1) \sum_{k=0}^{n-2} \frac{(n-2)!(k+2)}{(n-2-k)! n^{k+1}} \\ &= n-1. \end{aligned}$$

The last equation could be proved by induction.

Next we will study the change of hitting times when an edge is added or removed from a graph. Explicit formulas will follow rather naturally from (3.28). Note that (3.28) also holds true for multi or weighted graphs.

We use the following notations. Let G be a connected graph and $x, y \in V(G)$ are two distinct vertices such that x is not adjacent to y. Let G' be the graph obtained from G by adding an edge between x and y. Then $V(G) = V(G')$ and $E(G') = E(G) \cup \{xy\}$, where xy denotes the edge between x and y. Denote by $H(x,y)$ and $H'(x,y)$ the hitting times on G and G' respectively.

With the above setup. We will compute $H(a,b)$ and $H'(a,b)$ for distinct vertices $a, b \in V(G)$. The results will be separately stated in four cases.

1. $a = x, b = y$.
2. $a = x, b \neq y$.
3. $a \neq x, b = y$.
4. $\{a, b\} \cap \{x, y\} = \emptyset$.

Theorem 5.3.4. *For Case (1), namely $a = x, b = y$, we have*

$$\tau(G')H'(x,y) - \tau(G)H(x,y) = \tau(G/\{x,y\}).$$

Proof. By (5.4), we have

$$\tau(G)H(x,y) = \sum_{\substack{u \in V(G) \\ u \neq x}} d_u \sum_{\substack{P \in \mathscr{P}_G(x,u) \\ y \notin P}} \tau(G/\{P,y\}) + d_x \tau(G/\{x,y\})$$

and

$$\tau(G')H'(x,y) = \sum_{\substack{u \in V(G) \\ u \neq x}} d_u \sum_{\substack{P \in \mathscr{P}_G(x,u) \\ y \notin P}} \tau(G/\{P,y\}) + (d_x + 1)\tau(G/\{x,y\}).$$

Here d_u, d_x denote the degrees of vertices in G.

By subtracting the above two equations, we get the desired identity. □

Here we make an important remark. The well-known identity $\tau(G') = \tau(G) + \tau(G/\{x,y\})$ is the consequence of the simple fact that the spanning trees of G' could be divided into two categories: those with or without the edge xy. We will use similar identities throughout the following calculations.

Theorem 5.3.5. *For Case (2), namely $a = x, b \neq y$, we have*

$$\begin{aligned}
&\tau(G')H'(x,b) - \tau(G)H(x,b) \\
=&\tau(G/\{y,b\})H_{G/\{y,b\}}(x,\{y,b\}) + \tau(G/\{x,b\})H_{G/\{x,b\}}(y,\{x,b\}) \\
&+ \tau(G'/\{x,b\}) + \sum_{\substack{P \in \mathscr{P}_{G'}(x,y) \\ b \notin P}} \tau(G'/\{P,b\}).
\end{aligned}$$

Here $G/\{y,b\}$ is the graph obtained from G by merging y and b into a single vertex, which is denoted by $\{y,b\}$. Denote by $H_{G/\{y,b\}}(x,\{y,b\})$ the hitting time from x to $\{y,b\}$ on $G/\{y,b\}$. Similar definitions for $G/\{x,b\}$ and $H_{G/\{x,b\}}(y,\{x,b\})$. Note that $G/\{y,b\}$ and $G/\{x,b\}$ may have multi-edges.

Proof. By (5.4), we have

$$\tau(G)H(x,b) = \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(x,u)\\ b\notin P}} \tau(G/\{P,b\}) + d_x\tau(G/\{x,b\}) + d_y \sum_{\substack{P\in\mathscr{P}_G(x,y)\\ b\notin P}} \tau(G/\{P,b\})$$

and

$$\begin{aligned}\tau(G')H'(x,b) &= \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_{G'}(x,u)\\ b\notin P}} \tau(G'/\{P,b\}) + (d_x+1)\tau(G'/\{x,b\}) \\ &\quad + (d_y+1) \sum_{\substack{P\in\mathscr{P}_{G'}(x,y)\\ b\notin P}} \tau(G'/\{P,b\}) \\ &= \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(x,u)\\ b\notin P}} \tau(G'/\{P,b\}) + \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(y,u)\\ x\notin P, b\notin P}} \tau(G'/\{P,x,b\}) \\ &\quad + (d_x+1)\tau(G'/\{x,b\}) + (d_y+1) \sum_{\substack{P\in\mathscr{P}_{G'}(x,y)\\ b\notin P}} \tau(G'/\{P,b\}).\end{aligned}$$

Here d_u, d_x, d_y denote the degrees of vertices in G.

Subtract the above two equations,

$$\begin{aligned}&\tau(G')H'(x,b) - \tau(G)H(x,b) \\ &= \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(x,u)\\ y\notin P, b\notin P}} \tau(G/\{P,y,b\}) + \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(y,u)\\ x\notin P, b\notin P}} \tau(G/\{P,x,b\}) \\ &\quad + d_x\tau(G/\{x,y,b\}) + \tau(G'/\{x,b\}) + d_y\tau(G/\{x,y,b\}) + \sum_{\substack{P\in\mathscr{P}_{G'}(x,y)\\ b\notin P}} \tau(G'/\{P,b\}).\end{aligned}$$

Here we used some typical identities such as

$$\begin{aligned}&\sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(x,u)\\ b\notin P}} \tau(G'/\{P,b\}) \\ &= \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \left(\sum_{\substack{P\in\mathscr{P}_G(x,u)\\ y\in P, b\notin P}} \tau(G'/\{P,b\}) + \sum_{\substack{P\in\mathscr{P}_G(x,u)\\ y\notin P, b\notin P}} \tau(G'/\{P,b\}) \right)\end{aligned}$$

$$= \sum_{\substack{u\in V(G)\\u\neq x,u\neq y}} d_u \left(\sum_{\substack{P\in\mathscr{P}_G(x,u)\\y\in P,b\notin P}} \tau(G/\{P,b\}) + \sum_{\substack{P\in\mathscr{P}_G(x,u)\\y\notin P,b\notin P}} \Big(\tau(G/\{P,b\}) + \tau(G/\{P,y,b\})\Big)\right)$$

$$= \sum_{\substack{u\in V(G)\\u\neq x,u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(x,u)\\b\notin P}} \tau(G/\{P,b\}) + \sum_{\substack{u\in V(G)\\u\neq x,u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(x,u)\\y\notin P,b\notin P}} \tau(G/\{P,y,b\}).$$

Finally, it is not difficult to see that

$$\begin{aligned}&\tau(G/\{y,b\})H_{G/\{y,b\}}(x,\{y,b\})\\ =&\sum_{\substack{u\in V(G)\\u\neq x,u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(x,u)\\y\notin P,b\notin P}} \tau(G/\{P,y,b\}) + d_x\tau(G/\{x,y,b\})\end{aligned}$$

and

$$\begin{aligned}&\tau(G/\{y,b\})H_{G/\{y,b\}}(x,\{y,b\})\\ =&\sum_{\substack{u\in V(G)\\u\neq x,u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(y,u)\\x\notin P,b\notin P}} \tau(G/\{P,x,b\}) + d_y\tau(G/\{x,y,b\}).\end{aligned}$$

We get the desired identity. □

Theorem 5.3.6. *For Case (3), namely $a \neq x, b = y$, we have*

$$\begin{aligned}&\tau(G')H'(a,y) - \tau(G)H(a,y)\\ =&\tau(G/\{x,y\})H_{G/\{x,y\}}(a,\{x,y\}) + \sum_{\substack{P\in\mathscr{P}_G(a,x)\\y\notin P}} \tau(G/\{P,y\}).\end{aligned}$$

Proof. By (5.4), we have

$$\tau(G)H(a,y) = \sum_{\substack{u\in V(G)\\u\neq x,u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(a,u)\\y\notin P}} \tau(G/\{P,y\}) + d_x \sum_{\substack{P\in\mathscr{P}_G(a,x)\\y\notin P}} \tau(G/\{P,y\})$$

and

$$\begin{aligned}\tau(G')H'(a,y) =& \sum_{\substack{u\in V(G)\\u\neq x,u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_{G'}(a,u)\\y\notin P}} \tau(G'/\{P,y\}) + (d_x+1) \sum_{\substack{P\in\mathscr{P}_{G'}(a,x)\\y\notin P}} \tau(G'/\{P,y\})\\ =& \sum_{\substack{u\in V(G)\\u\neq x,u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(a,u)\\y\notin P}} \tau(G'/\{P,y\}) + (d_x+1) \sum_{\substack{P\in\mathscr{P}_G(a,x)\\y\notin P}} \tau(G/\{P,y\}).\end{aligned}$$

Here d_u, d_x denote the degrees of vertices in G.

Subtract the above two equations,

$$\begin{aligned}
&\tau(G')H'(x,b) - \tau(G)H(x,b) \\
=& \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in \mathscr{P}_G(a,u)\\ x\notin P, y\notin P}} \tau(G/\{P,x,y\}) + \sum_{\substack{P\in \mathscr{P}_G(a,x)\\ y\notin P}} \tau(G/\{P,y\}).
\end{aligned}$$

Finally, it is not difficult to see that

$$\tau(G/\{x,y\})H_{G/\{x,y\}}(a,\{x,y\}) = \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in \mathscr{P}_G(a,u)\\ x\notin P, y\notin P}} \tau(G/\{P,x,y\}).$$

We get the desired identity. □

Theorem 5.3.7. *For Case (4), namely $\{a,b\}\cap\{x,y\}=\emptyset$, we have*

$$\begin{aligned}
&\tau(G')H'(a,b) - \tau(G)H(a,b) \\
=&\tau(G/\{x,y\})H_{G/\{x,y\}}(a,b) + \sum_{\substack{P\in \mathscr{P}_G(a,x)\\ b\notin P}} \tau(G'/\{P,b\}) + \sum_{\substack{P\in \mathscr{P}_G(a,y)\\ b\notin P}} \tau(G'/\{P,b\}) \\
&+ \sum_{\substack{P\in \mathscr{P}_G(a,y)\\ b\notin P, x\notin P}} \tau(G/\{P,x,b\}) + \sum_{\substack{P\in \mathscr{P}_G(a,x)\\ b\notin P, y\notin P}} \tau(G/\{P,y,b\}).
\end{aligned}$$

Proof. By (5.4), we have

$$\begin{aligned}
\tau(G)H(a,b) =& \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in \mathscr{P}_G(a,u)\\ b\notin P}} \tau(G/\{P,b\}) + d_x \sum_{\substack{P\in \mathscr{P}_G(a,x)\\ b\notin P}} \tau(G/\{P,b\}) \\
&+ d_y \sum_{\substack{P\in \mathscr{P}_G(a,y)\\ b\notin P}} \tau(G/\{P,b\})
\end{aligned}$$

and

$$\begin{aligned}
\tau(G')H'(a,b) =& \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in \mathscr{P}_{G'}(a,u)\\ b\notin P}} \tau(G'/\{P,b\}) + (d_x+1) \sum_{\substack{P\in \mathscr{P}_{G'}(a,x)\\ b\notin P}} \tau(G'/\{P,b\}) \\
&+ (d_y+1) \sum_{\substack{P\in \mathscr{P}_{G'}(a,y)\\ b\notin P}} \tau(G'/\{P,b\}) \\
=& \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in \mathscr{P}_G(a,u)\\ b\notin P}} \tau(G'/\{P,b\}) + \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in \mathscr{P}_{G'}(a,u)\\ b\notin P, xy\in P}} \tau(G'/\{P,b\})
\end{aligned}$$

$$+ (d_x+1) \sum_{\substack{P\in\mathscr{P}_G(a,x)\\ b\notin P}} \tau(G'/\{P,b\}) + (d_x+1) \sum_{\substack{P\in\mathscr{P}_{G'}(a,x)\\ b\notin P, xy\in P}} \tau(G'/\{P,b\})$$

$$+ (d_y+1) \sum_{\substack{P\in\mathscr{P}_G(a,y)\\ b\notin P}} \tau(G'/\{P,b\}) + (d_y+1) \sum_{\substack{P\in\mathscr{P}_{G'}(a,y)\\ b\notin P, xy\in P}} \tau(G'/\{P,b\}).$$

Here d_u, d_x, d_y denote the degrees of vertices in G and $xy \in P$ means that P contains the edge xy.

Subtract the above two equations,

$$\begin{aligned}
&\tau(G')H'(x,b) - \tau(G)H(x,b)\\
=&\sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(a,u)\\ b\notin P, \{x,y\}\not\subset P}} \tau(G/\{P,b\}/\{x,y\}) + \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_{G'}(a,u)\\ b\notin P, xy\in P}} \tau(G'/\{P,b\})\\
&+ d_x \sum_{\substack{P\in\mathscr{P}_G(a,x)\\ b\notin P, y\notin P}} \tau(G/\{P,b\}/\{x,y\}) + \sum_{\substack{P\in\mathscr{P}_G(a,x)\\ b\notin P}} \tau(G'/\{P,b\})\\
&+ (d_x+1) \sum_{\substack{P\in\mathscr{P}_{G'}(a,x)\\ b\notin P, xy\in P}} \tau(G'/\{P,b\}) + d_y \sum_{\substack{P\in\mathscr{P}_G(a,y)\\ b\notin P, x\notin P}} \tau(G/\{P,b\}/\{x,y\})\\
&+ \sum_{\substack{P\in\mathscr{P}_G(a,y)\\ b\notin P}} \tau(G'/\{P,b\}) + (d_y+1) \sum_{\substack{P\in\mathscr{P}_{G'}(a,y)\\ b\notin P, xy\in P}} \tau(G'/\{P,b\}).
\end{aligned}$$

Here $\{x,y\} \not\subset P$ means that P does not pass both x and y. $G/\{P,b\}/\{x,y\}$ denotes the graph obtained from G by first contracting $\{P,b\}$ and then merging $\{x,y\}$.

Next we note that

$$\sum_{\substack{P\in\mathscr{P}_{G'}(a,x)\\ b\notin P, xy\in P}} \tau(G'/\{P,b\}) = \sum_{\substack{P\in\mathscr{P}_G(a,y)\\ b\notin P, x\notin P}} \tau(G/\{P,b\}/\{x,y\})$$

and

$$\sum_{\substack{P\in\mathscr{P}_{G'}(a,y)\\ b\notin P, xy\in P}} \tau(G'/\{P,b\}) = \sum_{\substack{P\in\mathscr{P}_G(a,x)\\ b\notin P, y\notin P}} \tau(G/\{P,b\}/\{x,y\}).$$

Finally, it is not difficult to see that

$$\begin{aligned}
&\tau(G/\{x,y\})H_{G/\{x,y\}}(a,b)\\
=&\sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_G(a,u)\\ b\notin P, \{x,y\}\not\subset P}} \tau(G/\{P,b\}/\{x,y\}) + \sum_{\substack{u\in V(G)\\ u\neq x, u\neq y}} d_u \sum_{\substack{P\in\mathscr{P}_{G'}(a,u)\\ b\notin P, xy\in P}} \tau(G'/\{P,b\})
\end{aligned}$$

$$+ (d_x + d_y) \sum_{\substack{P \in \mathscr{P}_G(a,x) \\ b \notin P, y \notin P}} \tau(G/\{P,b\}/\{x,y\}) + (d_x + d_y) \sum_{\substack{P \in \mathscr{P}_G(a,y) \\ b \notin P, x \notin P}} \tau(G/\{P,b\}/\{x,y\}).$$

We get the desired identity. □

We will present two examples when G is the path P_n and when G' is the complete graph K_n as testaments to the above formulas in Theorems 5.3.4-5.3.7.

Example 5.3.8. *Let $G = P_n$ be the path on n vertices $\{1, \ldots, n\}$, $n \geq 3$. Take $x = 1$ and $y = n$. Then $G' = C_n$ the circle on n vertices.*

In each case, we will denote by LHS the term $\tau(G')H'(a,b) - \tau(G)H(a,b)$ and denote by RHS the right-hand side of the corresponding formula.

Case (1). Namely $a = 1$ and $b = n$.

$$\begin{aligned} LHS &= \tau(C_n)H'(1,n) - \tau(P_n)H(1,n) \\ &= n(n-1) - (n-1)^2 \\ &= n - 1. \end{aligned}$$

On the other hand, $RHS = \tau(P_n/\{1,n\}) = n - 1$. Hence we verified $LHS = RHS$.

Case (2). Namely $a = 1$ and $2 \leq b \leq n-1$.

$$\begin{aligned} LHS &= \tau(C_n)H'(1,b) - \tau(P_n)H(1,b) \\ &= n(b-1)(n-b+1) - (b-1)^2 \\ &= (b-1)(n^2 + (1-b)n + 1 - b). \end{aligned}$$

On the other hand,

$$\begin{aligned} RHS =& \tau(P_n/\{n,b\})H_{P_n/\{n,b\}}(1,\{n,b\}) + \tau(P_n/\{1,b\})H_{P_n/\{1,b\}}(n,\{1,b\}) \\ &+ \tau(C_n/\{1,b\}) + \sum_{\substack{P \in \mathscr{P}_{C_n}(1,n) \\ b \notin P}} \tau(C_n/\{P,b\}) \\ =&(n-b)(b-1)^2 + (b-1)(n-b)^2 + (b-1)(n-b+1) + (b-1)(n-b) \\ =&(b-1)(n^2 + (1-b)n + 1 - b). \end{aligned}$$

Hence we verified $LHS = RHS$.

Case (3). Namely $2 \le a \le n-1$ and $b = n$.

$$\begin{aligned} LHS &= \tau(C_n)H'(a,n) - \tau(P_n)H(a,n) \\ &= n(n-a)a - \Big((n-1)^2 - (a-1)^2\Big) \\ &= (n-a)(an - n - a + 2). \end{aligned}$$

On the other hand,

$$\begin{aligned} RHS =& \tau(P_n/\{1,n\})H_{P_n/\{1,n\}}(a,\{1,n\}) + \sum_{\substack{P \in \mathscr{P}_{P_n}(a,1) \\ n \notin P}} \tau(P_n/\{P,n\}) \\ =& (n-1)(a-1)(n-a) + (n-a) \\ =& (n-a)(an - n - a + 2). \end{aligned}$$

Hence we verified $LHS = RHS$.

Case (4). Namely $2 \le a < b \le n-1$.

$$\begin{aligned} LHS &= \tau(C_n)H'(a,b) - \tau(P_n)H(a,b) \\ &= n(b-a)(n-b+a) - \Big((b-1)^2 - (a-1)^2\Big) \\ &= (b-a)(n^2 + (a-b)n + 2 - b - a). \end{aligned}$$

On the other hand,

$$\begin{aligned} RHS =& \tau(P_n/\{1,n\})H_{P_n/\{1,n\}}(a,b) + \sum_{\substack{P \in \mathscr{P}_{P_n}(a,1) \\ b \notin P}} \tau(C_n/\{P,b\}) + \sum_{\substack{P \in \mathscr{P}_{P_n}(a,n) \\ b \notin P}} \tau(C_n/\{P,b\}) \\ &+ \sum_{\substack{P \in \mathscr{P}_{P_n}(a,n) \\ b \notin P, 1 \notin P}} \tau(P_n/\{P,1,b\}) + \sum_{\substack{P \in \mathscr{P}_{P_n}(a,1) \\ b \notin P, n \notin P}} \tau(P_n/\{P,n,b\}) \\ =& (n-1)(b-a)(n-1+a-b) + (b-a)(n-b+1) + 0 + 0 + (b-a)(n-b) \\ =& (b-a)(n^2 + (a-b)n + 2 - b - a). \end{aligned}$$

Example 5.3.9. *Let $G' = K_n$ the complete graph on n vertices and G be the graph obtained by deleting an edge xy (keeping vertices x and y) from K_n. Take $x = 1$ and $y = 2$.*

By [4, Corollary 3.7], the hitting times on G are given by

$$H(1,2) = n+1, \quad H(1,3) = n-1-\frac{3}{n}, \quad H(3,1) = n, \quad H(3,4) = n-1-\frac{2}{n}.$$

Recall the following fact which will be used repeatedly. Denote by $K_n(s)$ be the graph obtained from K_n by merging s vertices into a single vertex. Then its number of spanning trees $\tau(K_n(s)) = s \cdot n^{n-s-1}$. In particular, when $s = 1$, we get $\tau(K_n) = n^{n-2}$. The number of spanning trees of G is

$$\begin{aligned}\tau(G) &= \tau(K_n) - \tau(K_n(2)) \\ &= n^{n-2} - 2n^{n-3} \\ &= n^{n-3}(n-2).\end{aligned}$$

Again we denote by LHS the term $\tau(G')H'(a,b) - \tau(G)H(a,b)$ and denote by RHS the right-hand side of the corresponding formula.

Case (1). Namely $a = 1$ and $b = 2$.

$$\begin{aligned}LHS &= \tau(K_n)H'(1,2) - \tau(G)H(1,2) \\ &= n^{n-2}(n-1) - n^{n-3}(n-2)(n+1) \\ &= 2n^{n-3}.\end{aligned}$$

On the other hand, $RHS = \tau(G/\{1,2\}) = \tau(K_n(2)) = 2n^{n-3}$. Hence we verified $LHS = RHS$.

Case (2). Namely $a = 1$ and $3 \le b \le n$.

$$\begin{aligned}LHS &= \tau(K_n)H'(1,b) - \tau(G)H(1,b) \\ &= n^{n-2}(n-1) - n^{n-3}(n-2)\left(n-1-\frac{3}{n}\right) \\ &= 2n^{n-2} + n^{n-3} - 6n^{n-4}.\end{aligned}$$

On the other hand,

$$\begin{aligned}RHS =&\tau(G/\{2,b\})H_{G/\{2,b\}}(1,\{2,b\}) + \tau(G/\{1,b\})H_{G/\{1,b\}}(2,\{1,b\})\\&+\tau(K_n/\{1,b\}) + \sum_{\substack{P\in\mathscr{P}_{K_n}(1,2)\\ b\notin P}}\tau(K_n/\{P,b\}).\end{aligned}$$

Let us calculate the first term by using (3.28)*.*

$$\begin{aligned}&\tau(G/\{2,b\})H_{G/\{2,b\}}(1,\{2,b\})\\=&(n-2)\tau(K_n(3)) + (n-1)\sum_{i=1}^{n-3}\binom{n-3}{i}i!\tau(K_n(i+3))\\=&(n-2)3n^{n-4} + (n-1)(n-3)n^{n-4}\\=&(n^2-n-3)n^{n-4}.\end{aligned}$$

The remaining terms of RHS are easy to calculate.

$$\begin{aligned}RHS =&(n^2-n-3)n^{n-4} + (n^2-n-3)n^{n-4} + 2n^{n-3}\\&+\sum_{i=0}^{n-3}\binom{n-3}{i}i!\tau(K_n(i+3))\\=&2(n^2-n-3)n^{n-4} + 2n^{n-3} + n^{n-3}\\=&2n^{n-2} + n^{n-3} - 6n^{n-4}.\end{aligned}$$

Hence we verified $LHS = RHS$.

Case (3). Namely $3 \le a \le n$ and $b = 2$.

$$\begin{aligned}LHS &= \tau(K_n)H'(a,2) - \tau(G)H(a,2)\\&= n^{n-2}(n-1) - n^{n-3}(n-2)n\\&= n^{n-2}.\end{aligned}$$

On the other hand,

$$RHS =\tau(G/\{1,2\})H_{G/\{1,2\}}(a,\{1,2\}) + \sum_{\substack{P\in\mathscr{P}_G(a,1)\\ 2\notin P}}\tau(G/\{P,2\})$$

Let us calculate the first term by using (3.28).

$$\tau(G/\{1,2\})H_{G/\{1,2\}}(a,\{1,2\}) = (n-1)\sum_{i=0}^{n-3}\binom{n-3}{i}i!\tau(K_n(i+3)) = (n-1)n^{n-3}.$$

Therefore

$$\begin{aligned} RHS =&(n-1)n^{n-3} + \sum_{i=0}^{n-3}\binom{n-3}{i}i!\tau(K_n(i+3)) \\ &= (n-1)n^{n-3} + n^{n-3} \\ &= n^{n-2}. \end{aligned}$$

Hence we verified $LHS = RHS$.

Case (4). Namely $3 \le a < b \le n$.

$$\begin{aligned} LHS &= \tau(K_n)H'(a,b) - \tau(G)H(a,b) \\ &= n^{n-2}(n-1) - n^{n-3}(n-2)\left(n-1-\frac{2}{n}\right) \\ &= 2n^{n-2} - 4n^{n-4}. \end{aligned}$$

On the other hand,

$$\begin{aligned} RHS =&\tau(G/\{1,2\})H_{G/\{1,2\}}(a,b) + \sum_{\substack{P\in\mathscr{P}_G(a,1) \\ b\notin P}}\tau(K_n/\{P,b\}) + \sum_{\substack{P\in\mathscr{P}_G(a,2) \\ b\notin P}}\tau(K_n/\{P,b\}) \\ &+ \sum_{\substack{P\in\mathscr{P}_G(a,2) \\ b\notin P, 1\notin P}}\tau(G/\{P,1,b\}) + \sum_{\substack{P\in\mathscr{P}_G(a,1) \\ b\notin P, 2\notin P}}\tau(G/\{P,2,b\}). \end{aligned}$$

Let us calculate $H_{G/\{1,2\}}(a,b)$ by the first step analysis. Let $u = H_{G/\{1,2\}}(a,b)$ and $v = H_{G/\{1,2\}}(\{1,2\},b)$. Then they satisfy the system of equations

$$\begin{cases} u = \frac{2}{n-1}v + \frac{n-4}{n-1}u + 1 \\ v = \frac{n-3}{n-2}u + 1 \end{cases}$$

The solution is $u = \frac{(n+1)(n-2)}{n}$ and $v = \frac{n^2-n-3}{n}$. Therefore

$$RHS =2n^{n-3}\frac{(n+1)(n-2)}{n}$$

$$
\begin{aligned}
&+ 2\left(\sum_{i=0}^{n-3}\binom{n-3}{i} i!\tau(K_n(i+3)) - \sum_{i=0}^{n-4}\binom{n-4}{i} i!\tau(K_n(i+4))\right)\\
&+ 2\sum_{i=0}^{n-4}\binom{n-4}{i} i!\tau(K_n(i+4))\\
=&2n^{n-4}(n+1)(n-2) + 2(n^{n-3} - n^{n-4}) + 2n^{n-4}\\
=&2n^{n-2} - 4n^{n-4}.
\end{aligned}
$$

Hence we verified $LHS = RHS$.

6.0 RANDOM WALK ON WEIGHTED GRAPHS

Random walks on general weighted graphs and their applications have been intensively studied in recent years. We refer the readers to [1, 4, 15, 19, 22] for some recent works.

Almost all of the above work on Chung-Yau invariants and their applications could be generalized to a weighted graph $G = (V, E)$ with edge weights $w_{xy} > 0$. We may assume that G has no multi-edges but may have a loop of weight w_{xx} at each vertex x. If there is no edge between x and y, we may take $w_{xy} = 0$. The weighted degree d_x of x is the sum of all w_{xy}, $y \in V$. The *volume* of a graph is $\mathrm{vol}(G) = \sum_{v \in V} d_v$.

A random walk on a weighted graph G is a Markov chain with transition probability $p_{xy} = w_{xy}/d_x$. If $w_{xx} \neq 0$, then walker may stay at the current vertex x, this is the so-called lazy random walk.

For a weighted graph G, denote by $\Omega(G)$ the set of spanning trees of G. Note that no matter whether G has loops, a spanning tree of G does not contain any loops. For $T \in \Omega(G)$, define the weight $w(T)$ of T to be $\prod_{e \in T} w_e$. The weighted counting of spanning trees $\tau(G)$ of G is defined by

$$\tau(G) = \sum_{T \in \Omega(G)} w(T).$$

6.1 HITTING TIMES OF WEIGHTED GRAPHS

The generalization of Chung-Yau invariants for weighted graphs is straightforward. For a weighted graph G, consider the following matrix

$$B(x,y) = \begin{cases} d_x^2 s + d_x - w_{xx} & \text{if } x = y, \\ d_x d_y s - w_{xy} & \text{if } x \sim y, \\ d_x d_y s & \text{otherwise,} \end{cases} \tag{6.1}$$

where s is a formal variable.

For any induced subgraph S of G, denote by B_S the principle submatrix of B on indices corresponding to the vertices of S, we define the Chung-Yau invariants $R(S)$ and $Z(S)$ by

$$\det B_S = R(S) + Z(S) \cdot s.$$

In particular, we have the following formula, which generalizes Theorem 3.3.4.

Theorem 6.1.1. *Let G be a connected weighted graph and $x, y \in V(G)$. Then*

$$H(x,y) = \frac{1}{\tau(G)} \sum_{u \in V(G)} d_u \sum_{\substack{P \in \mathscr{P}_G(x,u) \\ y \notin P}} \prod_{e \in E(P)} w_e R(G - \{P, y\}). \tag{6.2}$$

In fact, $R(G - \{P, y\}) = \tau(G/\{P, y\})$, where $G/\{P, y\}$ is obtained from G by contracting $\{P, y\}$ to a point.

Note that by studying Chung-Yau invariants for weighted graphs, we can prove analogues of Theorem 3.3.1 and its corollary the equation (3.27) for weighted graphs. Then the proof of (6.2) is similar to that of (3.28).

A weighted tree T is a tree whose edges are assigned positive weights. Note that usually a tree is defined to be a graph without cycles, but here we allow loops (i.e., edges connecting a vertex to itself) which will not affect our results.

Theorem 6.1.2. *Let x, y be two distinct vertices of a weighted tree T and denote by P_{xy} the path $[x = v_0, v_1, \ldots, v_{k-1}, v_k = y]$ connecting x to y. For any $v_i \in V(P_{xy})$, we denote by T_i the component of $T - E(P_{xy})$ that contains v_i and denote by $w_{i-1,i}$ the weight of the edge $v_{i-1}v_i$. Then the hitting time $H(x, y)$ is given by*

$$H(x,y) = \sum_{j=0}^{k-1} \left(\sum_{u \in T_j} d_u \right) \left(\sum_{i=j+1}^{k} \frac{1}{w_{i-1,i}} \right). \tag{6.3}$$

Proof. By (6.2), we have

$$\begin{aligned} H(x,y) &= \frac{1}{\tau(T)} \sum_{\substack{u \in V(P_{xy}) \\ u \neq y}} \sum_{v \in T_u} \left(d_v \prod_{e \in E(P_{xv})} w_e \tau(T/\{P_{xv}, b\}) \right) \\ &= \frac{1}{\prod_{e \in E(T)} w_e} \sum_{\substack{u \in V(P_{xy}) \\ u \neq y}} \sum_{v \in T_u} d_v \left(\prod_{e \in E(T)} w_e \right) \left(\sum_{e \in E(P_{uy})} \frac{1}{w_e} \right) \\ &= \sum_{j=0}^{k-1} \left(\sum_{u \in T_j} d_u \right) \left(\sum_{i=j+1}^{k} \frac{1}{w_{i-1,i}} \right). \end{aligned}$$

Note that in the last equation, $T/\{P_{xv}, b\}$ is a unicycle graph whose unique cycle comes from merging the two endpoints u and y of the path P_{uy}. □

The formula (6.3) should also hold for infinite but locally finite connected trees (with positive edge weights). Since an infinite (locally finite) graph can be considered as a limit of a sequence of finite graphs, the hitting time formula (6.2) is still valid as long as the limit exists.

The following two corollaries follow directly from (6.3).

Corollary 6.1.3. *Let x, y be two distinct vertices of a weighted tree T. Then $H(x, y) < \infty$ if and only if*

$$\sum_{u \in \mathscr{S}} d_u < \infty,$$

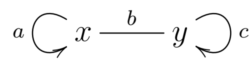
where $\mathscr{S} = \{u \in V(T) \mid$ There is a path from x to u not passing through $y\}$.

Corollary 6.1.4. *On the weighted one-dimensional lattice $\mathbb{Z}$,*

$$H(j, j+1) = \frac{\sum_{i \leq j} d_i}{w_{j,j+1}}.$$

The next example is about the calculation of hitting times on a weighted graph.

Example 6.1.5. *Let G be the two-vertex graph with an edge xy and loops at x and y. The edge weights a, b, c are as follows:*



We now compute the hitting time $H(x, y)$ by three methods.

(1) When the walker is at x, the probability to reach y in the next step is equal to $\frac{b}{a+b}$. Hence the expected number of steps to reach y is $\frac{a+b}{b}$. Thus $H(x, y) = \frac{a+b}{b}$.

(2) We apply (6.2). There is a unique spanning tree of G with weight b, hence $\tau(G) = b$. In the summation of (6.2), we only need to consider the trivial one-vertex path $\{x\}$. Then $H(x, y) = \frac{1}{b} d_x = \frac{a+b}{b}$.

(3) We apply (6.3) where $k = 1$. We immediately get $H(x, y) = \frac{a+b}{b}$.

We call a weighted graph G *reversible* if $H(x, y) = H(y, x)$ holds for any $x, y \in V(G)$. For simplicity, we assume that G has no loops, i.e., $w_{xx} = 0$, $\forall x \in V(G)$ and all edge weights of G are positive. It is interesting to study restrictions on edge weights for a reversible graph G.

Example 6.1.6. *For the 3-vertex path with positive weights a and b, it could never be reversible no matter how we adjust the values of a and b.*

Proof. We can set $w_{12} = a$, $w_{23} = b$, $\tau(G) = ab$. The corresponding graph matrix is

$$B = \begin{bmatrix} a^2 + a & a(a+b) - a & ab \\ a(a+b) - a & (a+b)^2 + (a+b) & (a+b)b - b \\ ab & (a+b)b - b & b^2 + b \end{bmatrix}$$

By (6.3), we have

$$H(1,2) = \frac{1}{ab}(ab)$$
$$H(2,1) = \frac{1}{ab}((a+b)b + b \cdot b \cdot 1)$$

If $H(1,2) = H(2,1)$, then $b = 0$, which contradict with $b > 0$. Hence, it is not a reversible graph no matter how we adjust values of a and b. $\square$

Example 6.1.7. *For the 3-cycle with positive weights $a, b, c > 0$, it is reversible if and only if $a = b = c$.*

Proof. We have $w_{13} = b$, $w_{12} = c$, $w_{23} = a$, $\tau(G) = ab + ac + bc$. The corresponding graph matrix is

$$B = \begin{bmatrix} (b+c)^2 + (b+c) & (b+c)(a+c) - c & (b+c)(a+b) - b \\ (b+c)(a+c) - c & (a+c)^2 + (a+c) & (a+c)(a+b) - c \\ (b+c)(a+b) - b & (a+c)(a+b) - a & (a+b)^2 + (a+b) \end{bmatrix}$$

By (6.2), we have

$$H(1,2) = \frac{1}{ab + ac + bc}((b+c)(a+b) + (a+b) \cdot b \cdot 1)$$
$$H(2,1) = \frac{1}{ab + ac + bc}((a+c)(a+b) + (a+b) \cdot a \cdot 1)$$

If $H(1,2) = H(2,1)$, then $a^2 = b^2$, thus $a = b$. Similarly, $H(1,3) = H(3,1)$ implies $a = c$. Therefore, a weighted 3-cycle is reversible if and only if $a = b = c$. $\square$

From the above example, it is natural to raise the following conjecture.

Conjecture 6.1.8 ([4]). *Let G be a weighted cycle on n vertices. Assume all edge weights of G are positive. Denote $w_{n,n+1} = w_{n,1}$.*

(i) If n is odd, then G is reversible if and only if there exists some $a > 0$ such that $w_{i,i+1} = a$ for all $1 \leq i \leq n$.

(ii) If n is even, then G is reversible if and only if there exist $a, b > 0$ such that $w_{1,2} = w_{3,4} = \cdots = w_{n-1,n} = a$ and $w_{2,3} = w_{4,5} = \cdots = w_{n,1} = b$.

The sufficiency of the above conjecture is clear. We have verified the above conjecture for $n \leq 4$ by writing a Mathematica program.

6.2 WEIGHT SCHEMES ON GRAPHS

Given a simple, connected, undirected graph G with n vertices, we may get a weighted graph by assigning a positive number w_e to each edge $e \in E(G)$. It is well-known that the hitting and cover times of a simple random walk on G (i.e. $w_e = 1$, $\forall e \in E(G)$) are upper bounded by $O(n^3)$. The work of [14] showed that if a token knows not only the degree of the current vertex it is on, but also the degrees of neighboring vertices, the hitting times are upper bounded by $O(n^2)$.

Definition 6.2.1. *In this section, we will denote by $d(u)$ the number of edges adjacent to a vertex u in G and d_u is still reserved for the total weights of edges adjacent to u.*

Recall the following Lemma 6.2.1 and Theorem 6.2.2.

Lemma 6.2.1 ([14]). *Let G be connected graph with n vertices and $u_0 = x, u_1, \ldots, u_l = y$ be a shortest path (achieving minimum l) connecting any two distinct vertices x and y. Then $\sum_{i=0}^{l} d(u_i) \leq 3n - 4$. More precisely,*

$$\sum_{i=0}^{l} d(u_i) \leq \begin{cases} 2n-2 & \text{if } l = 1, \\ 3n-l-3 & \text{if } l \geq 2. \end{cases}$$

Proof. First note that each vertex of $V(G)$ not lying on the shortest path can be connected to at most 3 vertices of the path. Also due to its shortestness, u_i, u_j are adjacent if and only if $|i-j| = 1$. Hence we have the claimed inequalities. □

Theorem 6.2.2 ([4]). *Let G be a connected weighted graph. Then*

$$H(x,y) \leq \max\{d_u \mid u \in \Gamma(y), u \neq y\} + \sum_{\substack{u \in V(G), u \neq y \\ u \notin \Gamma(y)}} d_u \min\big(d(x,y), d(u,y)\big), \tag{6.4}$$

where $\Gamma(y)$ is the set of vertices adjacent to y and $d(x,y)$ is defined by

$$d(x,y) = \min\left\{ \sum_{e \in E(P)} \frac{1}{w_e} \,\middle|\, P \in \mathscr{P}_G(x,y) \right\}.$$

In [4], the hitting times were estimated under three different weight schemes $w_{uv} = \frac{1}{\sqrt{d(u)d(v)}}$, $\frac{1}{\min\{d(u),d(v)\}}$ or $\frac{1}{\max\{d(u),d(v)\}}$ respectively. The leading terms of the bounds in Theorem 6.2.3 and Theorem 6.2.4 were obtained in [14, Thm. 2].

Theorem 6.2.3 ([4]). *Let G be a graph with assigned weights $w_{uv} = 1/\sqrt{d(u)d(v)}$ for each edge uv. Then the hitting time satisfies $H(x,y) \leq 3n^2 - 9n + \frac{15}{2}$.*

Proof. We have the estimates

$$d_u = \sum_{v\in\Gamma(u)} \frac{1}{\sqrt{d(u)d(v)}} \leq \frac{1}{2}\sum_{v\in\Gamma(u)}\left(\frac{1}{d(u)} + \frac{1}{d(v)}\right) \leq \frac{1}{2} + \frac{d(u)}{2} \leq \frac{n}{2}. \tag{6.5}$$

From

$$\sum_{u\in V(G)}\sum_{v\in\Gamma(u)} \frac{1}{2}\left(\frac{1}{d(u)} + \frac{1}{d(v)}\right) = n,$$

we have

$$\sum_{\substack{u\in V(G),u\neq y\\ u\notin\Gamma(y)}} d_u \leq \sum_{\substack{u\in V(G),u\neq y\\ u\notin\Gamma(y)}}\sum_{v\in\Gamma(u)} \frac{1}{2}\left(\frac{1}{d(u)} + \frac{1}{d(v)}\right) \leq n - 1 - \frac{d(y)}{2} \leq n - \frac{3}{2}. \tag{6.6}$$

Let $u_0 = x, u_1, \ldots, u_l = y$ be a shortest path (achieving minimum l) connecting x and y. Then

$$d(x,y) \leq \sum_{i=0}^{l-1}\sqrt{d(u_i)d(u_{i+1})} \leq \sum_{i=0}^{l-1}\frac{d(u_i) + d(u_{i+1})}{2} \leq 3n - 5. \tag{6.7}$$

The last inequality follows from Lemma 6.2.1. By Theorem 6.2.2, we have

$$H(x,y) \leq (3n-5)\left(n - \frac{3}{2}\right) + \frac{n}{2} = 3n^2 - 9n + \frac{15}{2},$$

as claimed. □

Theorem 6.2.4 ([4]). *Let G be a graph with assigned weights $w_{uv} = 1/\min\{d(u), d(v)\}$ for each edge uv. Then the hitting time satisfies $H(x,y) \leq 6n^2 - 18n + 14$.*

Theorem 6.2.5 ([4]). *Let G be a graph with assigned weights $w_{uv} = 1/\max\{d(u), d(v)\}$ for each edge uv. Then the hitting time satisfies $H(x,y) \leq 6n^2 - 23n + 23$.*

Among the above three theorems, it seems that the hitting times under the weights $w_{uv} = 1/\sqrt{d(u)d(v)}$ has the smallest upper bounds. On the other hand, it would be very interesting to know whether there are weights that would achieve upper bounds of hitting times $O(n^k)$ for some $k < 2$.

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