Random walks on quasi-1d infinite structures

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วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรดุษฎีบัณฑิต
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ในวิทยานิพนธ์ฉบับนี้ ผู้วิจัยศึกษาเชิงวิเคราะห์การเดินสุ่มบนโครงสร้างอนันต์กึ่งหนึ่งมิติที่พิจารณาว่าเป็นแบบจำลองของกระบวนการขนส่งในวัสดุกึ่งหนึ่งมิติ โดยขอบเขตของการศึกษาคือ การศึกษาพฤติกรรมเชิงเส้นกำกับของสมบัติเชิงสถิติพื้นฐานของการเดินสุ่มบนโครงสร้างดังกล่าว ซึ่งได้แก่ โมเมนต์ที่หนึ่งและโมเมนต์ที่สองของตำแหน่งตัวเดินในทิศทางตามแกนโครงสร้าง ความน่าจะเป็นของการกลับมายังจุดเริ่มต้น ความน่าจะเป็นของการไปยังตำแหน่งหนึ่งๆที่สนใจ เวลาเฉลี่ยของการไปยังตำแหน่งที่สนใจครั้งแรกแบบมีเงื่อนไข และจำนวนเฉลี่ยของตำแหน่งบนโครงสร้างที่แตกต่างกันที่ตัวเดินสุ่มเคยไปเยือน

ในส่วนแรกของวิทยานิพนธ์ ผู้วิจัยได้พัฒนาระเบียบวิธีการใหม่เพื่อวิเคราะห์สมบัติพื้นฐานเหล่านี้ โดยใช้แนวคิดของฟังก์ชันก่อกำเนิดและการแปลงฟูเรียร์ลาปลาซ และในส่วนที่เหลือของวิทยานิพนธ์จะเป็นการประยุกต์ใช้ระเบียบวิธีนี้ กับการเดินสุ่มบนแลตทิซกึ่งหนึ่งมิติแบบต่างๆ ได้แก่ แลตทิซหนึ่งมิติ แลตทิซแขนง แลตทิซบันได และแลตทิซทรงกระบอก รวมไปจนถึงการประยุกต์ใช้ที่เป็นไปได้ของผลลัพธ์ที่ได้จากการศึกษาการเดินสุ่มบนโครงสร้างต่างๆเหล่านี้

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In the present thesis a random walk on quasi-1d lattices as a model for transport processes on quasi-1d materials is analytically investigated. The scope of the present work is to shed light on the asymptotic behavior of basic statistical properties of the random walk on such structures including the first and the second moments of the walker location along the structure axis, the probability of return to the starting site, the probability of ever reach a given site, the conditional mean first-passage time to a given site and the expected number of distinct sites visited.

The first part of the thesis deals with developing a method for obtaining these basic properties by employing the concepts of generating functions and the Fourier-Laplace transform. Based on this developed method, in the remaining parts, the random walks on different quasi-1d lattices, i.e., a perfect-1d lattice, branched lattices, ladder lattices and cylindrical lattices, and their feasible applications are discussed.

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Srawut Sasom

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Introduction

A random walk often constitutes basic models for non-deterministic dynamics in diverse fields [1-3]. In physics, a number of studies of dynamical processes has exploited results of random walk models on various kinds of structures. For instance, the problem of the initial part of the low-temperature relaxation in the one-dimensional Ising model could be solved by employing the solution of a symmetric random walk on a one-dimensional lattice [4]. The transports of the excitation of a molecule on photosynthetic units and a particle inside spiny dendrites were modelled by a random walk on hexagonal lattices [5] and comb-like structures [6], respectively. In addition, even random walks on peculiar structures [7-10] can also motivate applications in diffusion in disordered media. It is thus evident that the problems of a random walk on structures of different topologies are still open and challenging. Among various structures, structures largely expanded in one direction than the others or the so-called quasi-one-dimensional (quasi-1d) structures, e.g., spiny dendrites, deoxyribonucleic acids (DNAs), polymers, carbon nanotubes and nanowires, have attracted very wide interests, because they play essential and ubiquitous roles in everyday life, and possess remarkable properties. To a certain extent, the study of a random walk on quasi-1d infinite structures could help in discussion of transport properties on such structures. Accordingly, this is the main motivation for this work.

Before we dive into our analysis, here is an introduction to the concept of random walks followed by an overview of examples of study on basic statistical properties of a random walk on different structures. In addition, according to our interest, before closing this chapter, we will mention some research relevant to transport processes in quasi-1d materials.

1.1 Random walks

1.1.1 History

The words “random walk” first appeared when Karl Pearson asked his question to the readers of Nature in 1905 [11] : “A man starts from a point O and walks L yards in a straight line; he then turns through any angle whatever and walks another L yards in a second straight line. He repeats this process n times. I require the probability that after n stretches he is at a distance between r and $r+dr$ from his starting point O.” This problem had in fact been studied in different contexts by several authors, e.g., Lord Rayleigh [12] who studied the composition of n iso-periodic vibrations of unit amplitude and of phases distributed at random in 1899, Bachelier [13] who proposed a random walk model of the stock market in 1900, and Einstein [14] who treated the motion of elements suspended in static liquids in the same year Pearson formulated the problem. This shows that the concept of random walks is related to numerous physical processes. Consequently, many authors put their efforts into analysis of various aspects of the random walk problems, e.g., Kluyver [15] who furnished a complete solution to the Pearson’s question, and Smoluchowski [16] who was the first to consider the problem of the restricted random walk – the random walk with the presence of reflecting and absorbing barriers. In the most general form, the problems were formulated by Markov [17] who outlined a general method of solutions.

Over the years the concept of random walks has found extensive application in diverse fields. For instance, it was applied to many problems in economics such as the ruin theory of insurance companies, growth and inequality processes and the dynamics of prices on financial markets [18]. The various areas of computer science have also exploited the random walk concept, for instance, recommender system, computer vision and network embedding [19]. In biology, random walks were used to describe the movement, the dispersal and the population redistribution of animals and micro-organisms [20]. In chemistry, particle diffusions with the presence of reactions in crowded media were studied by random walk models as well [21], and in physics persistent random walks of charged particles across magnetic field lines have been discussed recently [22].

1.1.2 General statement and formulation

The simplest definition of a random walk is a sum of random vectors:

$$\vec{x} = \vec{r}_1 + \vec{r}_2 + \ldots + \vec{r}_n \tag{1}$$

where $\vec{x}$ is the position of a walker after n steps and the random vector $\vec{r}_i$ represents the displacement at the ith step. The rigorous mathematical definition and the mathematical problems can be found in the book by Spitzer [23]. To illustrate this definition, let us go back to Pearson's question. In this question, the random vector $\vec{r}_i$ is the 2-d random vector with fixed magnitude L and random angle θ_i uniformly distributed over 0 to 2π, i.e., $\vec{r}_i = L\cos\theta_i\hat{x}_1 + L\sin\theta_i\hat{x}_2$ for $i = 1, 2, 3, \ldots, n$, and the probability distribution function (PDF) $\wp\left(|\vec{x}|\right)_n$ to find the walker at the nth step at points with distance $|\vec{x}|$ from the starting point was required.

For general random walk models, one may ask this basic question of the theory of random walks in a more general way: For given the characteristics of the transition of a random walker, what is the probability of the walker being found at a certain region at certain time? or what is the probability that a certain region is occupied by the walker at certain time? These two slightly different questions originate two key complimentary approaches to the statistical description of the random walk models. Although having different mathematical apparatus and terminologies, the two approaches are closely related and their exact equivalence can be demonstrated in some cases.

The first approach, often called the generating function formalism (GFF), is based on the concept of generating functions and the Fourier-Laplace transform. This approach is commonly employed to treat the problems of random walks if certain recursive relations play a fundamental role in describing the dynamics of walkers, and the models may possess the spatial and the temporal homogeneities.

To see this, let us consider a random walk on lattices due to Montroll and Weiss [24]. It is assumed that the model possesses the spatial homogeneity in a sense that the walker can take an instantaneous step of displacement $\Delta\vec{x}$ from the present site to the neighboring sites with probabilities $p\left(\Delta\vec{x}\right)$, which are independent of the past position. It also possesses the temporal homogeneity, which

means that the walker steps are taken at random times, $t_1, t_2, \ldots$ such that the times between steps $t_i' = t_i - t_{i-1}$ are independent to each other and have a common PDF $\psi(t_i')$ for $0 < t_i' < \infty$. These probabilities satisfy the normalization conditions: $\int_0^\infty \psi(t')\,dt' = 1$ and $\sum_{\Delta\vec{x}} p(\Delta\vec{x}) = 1$ where the sum is over all neighboring sites.

Consequently, the probability $\wp(\vec{x},t)$ that the walker is at a site $\vec{x}$ at time t, given that the walker started at the origin $\vec{x} = 0$, can be expressed in the form

$$\wp(\vec{x},t) = \int_0^t \left(\sum_{n=0}^{\infty} \wp(\vec{x})_n \psi(t')_n \right) \Psi(t-t')\,dt'. \tag{2}$$

$\wp(\vec{x})_n$ is the probability of the walker being at the site $\vec{x}$ at the nth step. It obeys the recursive relation, i.e., Chapman–Kolmogorov equation,

$$\wp(\vec{x})_n = \delta_{n,0}\delta_{\vec{x},0} + \sum_{\vec{x}'} p(\vec{x}-\vec{x}')\wp(\vec{x}')_{n-1} \tag{3}$$

where $\delta_{a,b}$ denotes the Kronecker delta and the sum is now over all sites on the structure. In turn, the term $\psi(t)_n\,dt$ is the probability for the occurrence of the nth step at time t, which satisfies the recursive relation

$$\psi(t)_n = \int_0^t \psi(t')_{n-1}\psi(t-t')\,dt' \tag{4}$$

where $\psi(t)_0 = \delta(t)$ and n is a natural number. The probability $\Psi(t) \equiv \int_t^\infty \psi(t')\,dt'$ is the so-called survival probability on a site, the probability that the waiting time on a site exceeds t. In short, the probability $\wp(\vec{x},t)$ can be considered as the sum of the probabilities that the walker makes a jump to a given site $\vec{x}$ at different steps and times, provided that the walker pauses movement at time t' until time t after its arrival to the site $\vec{x}$ at time t'.

From the convolution theorems of Fourier and Laplace transforms, we can turn the probability $\wp(\vec{x},t)$ in equation (2) to its Fourier-Laplace representation,

$$\tilde{\wp}^*(\vec{k},s) = \frac{1-\psi^*(s)}{s}\tilde{\wp}\left(\vec{k};\psi^*(s)\right) \tag{5}$$

where $\tilde{\wp}^*(\vec{k},s) \equiv \int_0^\infty \left(\sum_{\vec{x}} \wp(\vec{x},t) e^{i\vec{k}\cdot\vec{x}} \right) e^{-st}dt$ is the Fourier-Laplace transform of $\wp(\vec{x},t)$ and $\psi^*(s) \equiv \int_0^\infty \psi(t)e^{-st}dt$ is the Laplace transform of $\psi(t)$. In turn, the term

$\tilde{\wp}\left(\vec{k};\psi^*(s)\right)$ is the Fourier transform of the generating function $\wp(\vec{x};\xi)\equiv\sum_{n=0}^{\infty}\wp(\vec{x})_n\,\xi^n$, i.e., $\tilde{\wp}\left(\vec{k};\xi\right)\equiv\sum_{\vec{x}}\wp(\vec{x};\xi)e^{i\vec{k}\bullet\vec{x}}$, with ξ substituted by $\psi^*(s)$. From equation (3), it is not hard to show that $\tilde{\wp}\left(\vec{k};\xi\right)=\left(1-\xi\bar{p}\left(\vec{k}\right)\right)^{-1}$ where $\bar{p}\left(\vec{k}\right)\equiv\sum_{\Delta\vec{x}}p(\Delta\vec{x})e^{i\vec{k}\bullet\Delta\vec{x}}$ with the summation over all neighboring sites, and equation (5) thus takes a simple form,

$$\tilde{\wp}^*\left(\vec{k},s\right)=\frac{1-\psi^*(s)}{s\left(1-\psi^*(s)\,\bar{p}\left(\vec{k}\right)\right)}.$$

Therefore, the probability $\wp(\vec{x},t)$ can be calculated by performing the inverse Fourier-Laplace transform of $\tilde{\wp}^*\left(\vec{k},s\right)$. In addition, as we shall see later, the Fourier-Laplace transform $\tilde{\wp}^*\left(\vec{k},s\right)$ itself encodes other incredibly important properties of a random walk.

On the other hand, when models cannot be formulated from the recursive relations and the spatial homogeneity no longer holds, one may tackle the problems by the second approach, a master equation technique (MET) (see, e.g., [1] and [3]). For this technique, $\wp(\vec{x},t)$ is denoted as the probability that a given site $\vec{x}$ is occupied by a walker at time t, and its rate of change equals to the sum of the gain and the loss fluxes,

$$\frac{\partial}{\partial t}\wp(\vec{x},t)=\int_0^t\left[\sum_{\vec{x}'}p(\vec{x},\vec{x}';t-t')\wp(\vec{x}',t')-\sum_{\vec{x}'}p(\vec{x}',\vec{x};t-t')\wp(\vec{x},t')\right]dt' \qquad (6)$$

where the term $p(\vec{x},\vec{x}';t-t')$ is the transition probability rate for going from $\vec{x}'$ to $\vec{x}$ in time interval $t-t'$. This equation is known as the generalized master equation. Note that, in the spatial continuum limit, the sums become the integrals.

Unfortunately, in general, it is almost impossible to find the explicit form of the probability $\wp(\vec{x},t)$ from performing the inverse Fourier-Laplace transform of equation (5) or solving the integro-differential equation (6). Nevertheless, it has been shown [10] that, for a broad class of random walks, the asymptotic behavior of the probability $\wp(|\vec{x}|,t)$ to find a random walker at time t at points with distance $|\vec{x}|$ from the starting point $|\vec{x}|=0$ obeys the scaling collapse

$$\wp\left(|\vec{x}|,t\right) \sim t^{-\left(\frac{d_f}{d_w}\right)} f\left(\frac{|\vec{x}|}{t^{1/d_w}}\right) \tag{7}$$

with the scaling variable $|\vec{x}|/t^{1/d_w}$, where the parameters d_f and d_w are determined by the symmetries of the model and the geometric characteristics of the underlying structure. On lattices with translational invariance in any k-dimensional Euclidean space (k-d in short), it has been found that $d_f = k$, $d_w = 2$ and the function $f(\cdot)$ is a Gaussian scaling function. It is worth to note that the scaling collapse (7) is also valid when the underlying structure is a fractal.

Aside from being central in studying the probability $\wp\left(\vec{x},t\right)$ of random walks, GFF and MET also enable us to derive many other subtle and useful random walk properties. To demonstrate this statement, in the next section, we will introduce several works, which exploit the ideas of MET (Subsection 1.2.1 – 1.2.3) and GFF (Subsection 1.2.4 – 1.2.8) to study basic properties of a random walk on different structures.

1.2 Random walks on different structures

1.2.1 The random walk on complex networks

A complex network, a graph with non-trivial topological features (see, e.g., Figure 1), is a structure able to reproduce certain features of real-world networks, e.g., computer networks, biological networks, technological networks, brain networks, climate networks and social networks. Transports on this kind of networks can thus be described by a random walk on complex networks.

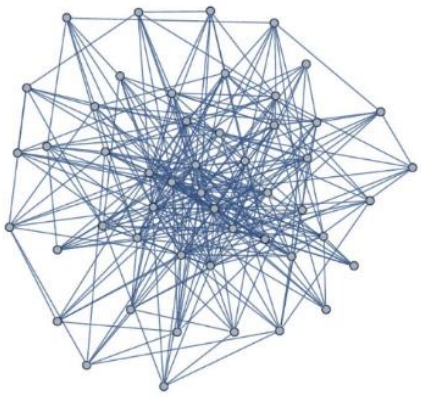


Figure 1. An example of complex networks, a Baraba´si–Albert graph [25]

One of the important functions used to describe the non-trivial topological features of complex networks is the degree distribution $P(k)$ - the fraction of nodes in a network with degree k. According to the conventional classification, complex networks are denominated by the behavior of the corresponding degree distributions. For example, a complex network is called a scale-free network or a growing exponential network when the degree distribution $P(k)$ follows the power law decay function in the continuous degree approximation, i.e., $P(k) \sim \text{constant} \times k^{-\gamma}$ for $2 < \gamma < 3$, or it is in the form of the exponential decay function, i.e., $P(k) = e^{1-k/m}/m$ where a counting number m is a minimum degree and $k \geq m$.

The random walk exploration on both types of complex networks was studied by Baronchelli, Catanzaro and Pastor-Satorras [26]. It was described through the coverage $\langle S \rangle(t)$, defined as the expected number of distinct nodes visited by a walker at time t, averaged for different random walks starting from different nodes. The coverage can be expressed as the weighted sum of the coverage spectrum $s_k(t)$ defined as the fraction of nodes of degree k visited by the random walker at least once. In other words, $\langle S \rangle(t) = N \sum_k P(k) s_k(t)$ where the complex network is composed of different N nodes. The evolution of the coverage spectrum $s_k(t)$ is described by the following differential equation,

$$\frac{\partial s_k(t)}{\partial t} = \left(k \sum_{k'} \frac{P(k'|k)}{k'} \rho_{k'}(t) \right) \left(1 - s_k(t)\right). \tag{8}$$

In words, the rate of change of the coverage spectrum equals to the multiplication of the gain flux of the probability that nodes of degree k host the random walker at time t (the first parentheses) and the fraction of nodes of degree k never visited by the walker (the second parentheses). As mentioned earlier, from the idea of MET, the sum of the gain flux and the loss flux is equal to the rate of change of the corresponding probability. Hence, the probability $\rho_k(t)$, which nodes of degree k host the random walker at time t, reads

$$\frac{\partial \rho_k(t)}{\partial t} = -\rho_k(t) + k \sum_{k'} \frac{P(k'|k)}{k'} \rho_{k'}(t) \tag{9}$$

where $P(k'|k)$ is defined as the probability that a node of degree k is connected to another node of degree k'.

The authors found that, from equations (8) and (9), in certain limits, the coverage spectrum of wide range of complex network models obeys the scaling law

$$s_k(t) = 1 - \exp\left(-\frac{kt}{\langle k\rangle N}\right) \tag{10}$$

which leads to the general scaling expression of the coverage $\langle S\rangle(t)$,

$$\frac{\langle S\rangle(t)}{N} = 1 - \sum_k P(k)\exp\left(-\frac{kt}{\langle k\rangle N}\right) \tag{11}$$

where $\langle k\rangle \equiv \sum_k kP(k)$ is the average of degrees.

From this result, it is immediately seen that, for finite complex network models, $N < \infty$, the random walks eventually visit all nodes of networks, $\langle S\rangle(t) \sim N$. The scaling expressions of the coverage $\langle S\rangle(t)$ for scale-free networks and growing exponential networks were respectively cast into the following forms:

$$\frac{\langle S\rangle(t)}{N} = 1 - (\gamma - 1)E_\gamma\left(\frac{mt}{\langle k\rangle N}\right) \tag{12}$$

where $E_\gamma(z)$ is the exponential integral function for $2 < \gamma < 3$, and

$$\frac{\langle S\rangle(t)}{N} = 1 - \frac{e^{-mt/\langle k\rangle N}}{1 + mt/\langle k\rangle N}. \tag{13}$$

1.2.2 The random walk on fractals

Fractals have drawn the widespread interest from many authors because of the self-similarity of the structures and the realization that such structures or approximations to them can be found everywhere in natural and artificial structures (see, e.g., [27] and [28]). The examples include percolations, polymers, surfaces in turbulent flows and geometrical optics. The geometrical characteristics of fractals are roughly determined by an index called a fractal dimension d_f, which is the same index appeared in equation (7), and it is defined by

$$d_f = \frac{\log(\text{number of relication})}{\log(\text{magnification})}. \tag{14}$$

Note that although there are many ways of introducing this index, these different ways are all related to each other. To clarify this definition, let us consider an

example, the Sierpinski gasket in 2-d. The first three stages in the construction of this self-similar structure are shown in Figure 2. It begins with one equilateral triangle. As you can see, subsequently, there are 3 copies of the original triangle constructed, and each of them needs to be magnified by the factor 2 to restore the original scale. The process is continued infinitely. Therefore, the fractal dimension of the Sierpinski gasket is $d_f = \frac{\log 3}{\log 2}$ which is a non-integer. The Sierpinski gasket can be generalized to a fractal in k-d, and its fractal dimension is $d_f = \frac{\log(k+1)}{\log 2}$ (see [29] for more details).

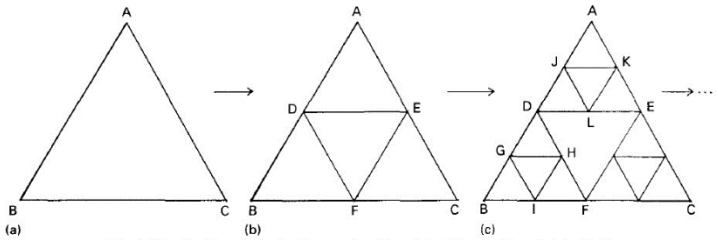


Figure 2. The several iterated processes to construct the Sierpinski gasket in 2-d [29].

In what follows, a summary, which is mentioned in the article of Balakrishnan [29], is given of some of results for the random walk on fractals. A fractal is a non-differentiable structure so the probability to find a walker at certain time at sites with certain distance from its starting site is expected to be non-differentiable function. However, a coarse-graining procedure enables us to define an "envelope" function $\wp(|\vec{x}|,t)$ that satisfies a differential equation, which can be derived from the generalized master equation,

$$\frac{\partial}{\partial t}\wp(|\vec{x}|,t) = \frac{K_0}{|\vec{x}|^{d_f-1}}\frac{\partial}{\partial|\vec{x}|}\left[|\vec{x}|^{d_f+1-d_w}\frac{\partial}{\partial|\vec{x}|}\wp(|\vec{x}|,t)\right] \tag{15}$$

where d_w, which is the same index appeared in equation (7), is an index characterizing the random motion of the walker. This index is also known as the random walk dimension. For $k \geq 2$, for regular lattices embedded in Euclidean space

of k-d, this index is always equal to 2, while, for the Sierpinski gasket in k-d, $d_w = \frac{\log(k+3)}{\log 2} > 2$.

For the spherically symmetric initial condition, the asymptotic form of the solution of equation (15) is

$$\wp(|\vec{x}|,t) \propto t^{-\left(\frac{d_f}{d_w}\right)} \exp\left(-\left(|\vec{x}|/t^{1/d_w}\right)^{d_w}\right), \tag{16}$$

which obeys the scaling form (7). From this result, one of basic random walk properties is immediate, i.e., the asymptotic form of the probability $\wp(0,t)$ of return to the starting site at time t, $\wp(0,t) \propto t^{-\left(\frac{d_f}{d_w}\right)}$. Furthermore, the relation (16) leads us to the characteristic index dependence of other physical quantities in the problems of random walks, e.g., the mean first-passage time $\tau(|\vec{x}|)$ of a walker being at sites with distance $|\vec{x}|$ from its starting site, $\tau(|\vec{x}|) \propto |\vec{x}|^{d_w}$ as the distance $|\vec{x}|$ is large, and the expected number $\langle S\rangle(t)$ of distinct sites visited, $\langle S\rangle(t) \propto t^{d_f/d_w}$ for $0 < d_f < 2$. In addition, it was pointed out that the walker diffusion on the Sierpinski gasket in k-d is in the subdiffusive regime, i.e., the second moment $\left\langle |\vec{x}|^2 \right\rangle(t) \equiv \int_0^\infty |\vec{x}|^2 \wp(|\vec{x}|,t) d|\vec{x}|$ behaves like t^{2/d_w} at large times, for $k > 1$.

1.2.3 The random walk on comb structures

A comb model was first proposed at roughly the same time by Goldhirsch and Gefen [30] and by Weiss and Havlin [31], as a basic model able to reproduce certain features of transport on a fractal medium and a percolation cluster. They have been the starting point for many successive developments on the problem of random walks on comb-like structures [7, 32-36]. The simplest comb structure, shown in Figure 3, consists of a principal axis, called the backbone, and identical branches attached to each site on the backbone.

Mendez, Iomin, Campos and Horsthemke [34] studied the continuous time random walks on this simplest comb structure and presented a generic method, which is based on MET, to obtain the random walk transport properties. They restricted themselves to the so-called Polya walk, a walk in which steps to

neighboring sites on a structure only are allowed. It is assumed that the walker takes symmetrically steps along the backbone, but the steps along branches may be biased with probability p. For example, when $p > 0.5$, the walker may likely move away from the backbone along a branch. In addition, when the walker arrives at any site on the structure, it waits for a random time t with a common PDF $\psi_0(t)$.

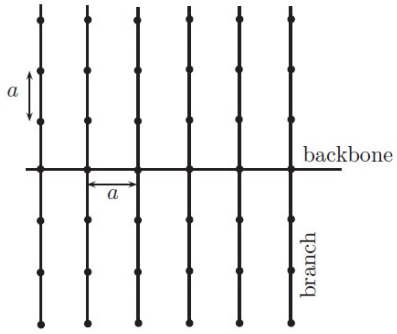


Figure 3. A comb structure consisting of the backbone and branches where a is the distance between two neighboring sites [34].

The authors found that the motion of the walker on the comb can be reduced to the effective motion along a one-dimensional lattice, corresponding to the backbone only. For this reduced model, the probability $\wp(x,t)$ of finding the walker at a site x on the backbone at time t can be derived from the generalized master equation,

$$\frac{\partial}{\partial t}\wp(x,t) = \int_0^t \left[\sum_{x'=-\infty}^{\infty} p\left(x-x'\right)\wp\left(x',t'\right) - \wp(x,t') \right] K\left(t-t'\right)dt' \tag{17}$$

where $p(\Delta x) \equiv \frac{1}{2}\delta_{\Delta x,a} + \frac{1}{2}\delta_{\Delta x,-a}$ represents the single-step transition probability, $K(t)$ is the memory kernel related to the PDF $\psi(t)$ of effective waiting time via its Laplace transform, $K^*(s) = \frac{s\psi^*(s)}{1-\psi^*(s)}$. The authors could derive an exact analytical expression for $\psi(t)$ of the random walk dynamics on the backbone in terms of the mesoscopic characteristics of the random walk on the comb, namely the PDF $\psi_0(t)$ of the local waiting time, the probability p, and the length N of branches,

$$\psi^*(s)=\frac{\psi_0^*(s)}{2-\dfrac{(1-p)\left(\psi_0^*(s)\right)^2}{1-(1-p)\psi_0^*(s)G\left(p,N,\psi_0^*(s)\right)}} \tag{18}$$

where $G\left(p,N,\psi_0^*(s)\right)$ is a certain complicated function (see [34] for more details).

From this result and the definitions of important parameters $0<\nu\leq 1$ and $t_0>0$ via the asymptotic form of the Laplace transform $\psi^*(s)$, $\psi^*(s)\sim 1-(t_0 s)^\nu$ as $s\to 0^+$, the authors could determine the asymptotic form of the second moment $\left\langle x^2\right\rangle(t)$ of the walker location along the backbone. For the comb with finite-length branches, $N<\infty$,

$$\left\langle x^2\right\rangle(t)\sim 2Dt_0\frac{(t/t_0)^\nu}{\Gamma(1+\nu)} \tag{19}$$

where $D\equiv\dfrac{a^2}{2t_0}\dfrac{2p-1}{2(1-p)^{1-N}p^N+4p-3}$ is called the diffusion coefficient, a is the distance between neighboring sites and $\Gamma(z)$ is the gamma function. On the other hand, for the comb with infinite-length branches, the random walks can display three different transport regimes depending on the degree p of bias on branches,

$$\left\langle x^2\right\rangle(t)\sim\begin{cases}\dfrac{a^2(2p-1)}{\Gamma(1+\nu)(4p-3)}\left(\dfrac{t}{t_0}\right)^\nu & ,p<0.5\\ \dfrac{a^2}{\sqrt{2}\Gamma(1+\nu/2)}\left(\dfrac{t}{t_0}\right)^{\nu/2} & ,p=0.5\\ \dfrac{a^2q(2p-1)}{\left(4p^2-3p+1\right)}\mu(t/t_0) & ,p>0.5\end{cases} \tag{20}$$

where the function $\mu(z)$ is expressed in term of the generalized Mittag-Leffler function $E_{\alpha,\beta}(z)$.

1.2.4 The random walk on arbitrary dimensional comb lattices

Although the simplest comb structure is a simple caricature of various types of branched structures, it does not exhaust the whole variety of cases. Therefore, Illien and Benichou put their focus on the generalization of the simplest comb model [7]. The generalization is a random walk on arbitrary dimensional comb lattices. Illustrations of these structures can be seen in Figure 4. In their work, it was assumed

that a walker located at any site $\vec{x}=(x_1,x_2,x_3,...,x_k)$ on a k-d comb takes symmetrically an instantaneous step to the neighboring sites with probabilities $1/\nu(\vec{x})$ where $\nu(\vec{x})$ is the number of neighboring site of the site $\vec{x}$. In addition, unlike the preceding model, this model is the discrete-time random walk, the walker steps are taken at certain times instead of random times.

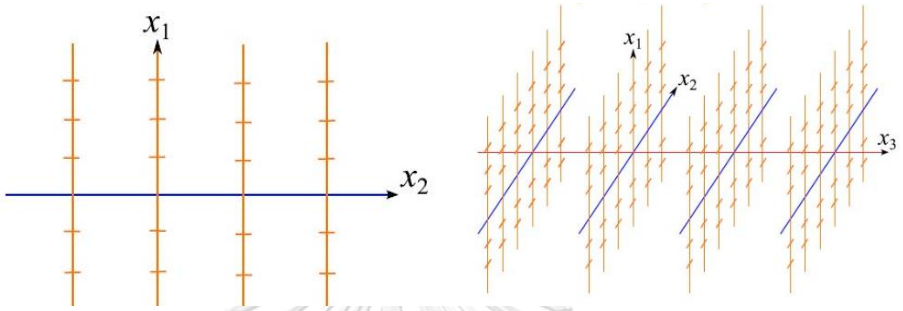


Figure 4. The structures of the 2-d (left) and 3-d (right) combs [7]. The line coincides with the x_k axis is called the primary backbone.

It is obvious that the models do not have the spatial homogeneity, but the following recursive relation is still helpful,

$$\wp(\vec{x}\,|\,\vec{x}_0)_n=\delta_{n,0}\delta_{\vec{x},\vec{x}_0}+\sum_{n'=0}^{n}\wp(\vec{x}\,|\,\vec{x})_{n'}\mathcal{F}(\vec{x}\,|\,\vec{x}_0)_{n-n'}. \tag{21}$$

The idea is: The probability $\wp(\vec{x}\,|\,\vec{x}_0)_n$ of the walker being at a site $\vec{x}$ at the nth step, given that it initiated at a site $\vec{x}_0$, is equal to the sum of all probabilities that the walker is at that site for the first time after walking $n-n'$ steps and, the rest of its walk n', it can go anywhere on the structure but eventually it must be at that site. In addition, the comb lattices are loopless structures, so two arbitrary sites $\vec{x}$ and $\vec{x}_0$ are connected to each other with a unique path. This property implies that the generating function $\mathcal{F}(\vec{x}\,|\,\vec{x}_0;\xi)\equiv\sum_{n=0}^{\infty}\mathcal{F}(\vec{x}\,|\,\vec{x}_0)_n\,\xi^n$ of the conditional first-passage probabilities $\mathcal{F}(\vec{x}\,|\,\vec{x}_0)_n$ is sparable,

$$\mathcal{F}(\vec{x}\,|\,\vec{x}_0;\xi)=\mathcal{F}(\vec{x}\,|\,\vec{x}_1;\xi)\mathcal{F}(\vec{x}_1\,|\,\vec{x}_0;\xi) \tag{22}$$

where $\vec{x}_1$ is any site belonging to the path. Furthermore, it has been proven that the model possesses the reversibility,

$$\frac{1}{\nu(\vec{x})}\wp(\vec{x}\,|\,\vec{x}_0;\xi)=\frac{1}{\nu(\vec{x}_0)}\wp(\vec{x}_0\,|\,\vec{x};\xi) \tag{23}$$

where $\wp(\vec{x}\,|\,\vec{x}_0;\xi)\equiv\sum_{n=0}^{\infty}\wp(\vec{x}\,|\,\vec{x}_0)_n\,\xi^n$.

Altogether, Illien and Benichou could find the explicit form of the generating function $\wp(\vec{x}\,|\,0;\xi)$ of the conditional probability $\wp(\vec{x}\,|\,0)_n$ that the walker is found at a site $\vec{x}$ at the nth step knowing that at the 0th step it was at the starting site O, a certain common site of the lines coinciding with the axes.

$$\wp(\vec{x}\,|\,0;\xi)=\frac{\nu(\vec{x})}{2k}G_k(\xi)\prod_{j=1}^{k}f_j(\xi)^{|x_j|} \tag{24}$$

where, for $j=2,3,4,\ldots,k$, $f_j(\xi)=\frac{j}{\xi}-\sum_{i=1}^{j-1}f_i(\xi)-\sqrt{\left(\frac{j}{\xi}-\sum_{i=1}^{j-1}f_i(\xi)\right)^2-1}$ and

$G_j(\xi)=j\left(\left(1+\frac{j-1}{G_{j-1}(\xi)}\right)^2-\xi^2\right)^{-1/2}$ with $f_1(\xi)=\frac{1-\sqrt{1-\xi^2}}{\xi}$ and $G_1(\xi)=\frac{1}{\sqrt{1-\xi^2}}$.

Consider the second moment of the random walker along the primary backbone of a k-d comb after n steps, which is defined by $\langle x_k^2\rangle_n\equiv\sum_{\vec{x}}x_k^2\wp(\vec{x}\,|\,0)_n$. It can also be calculated from the second derivative of the Fourier transform $\tilde{\wp}(\vec{k}\,|\,0;\xi)\equiv\sum_{\vec{x}}e^{i\vec{k}\cdot\vec{x}}\wp(\vec{x}\,|\,0;\xi)$ with respect to k_k evaluating at $\vec{k}=0$, i.e., $\langle x_k^2\rangle(\xi)=-\frac{\partial^2}{\partial k_k^2}\tilde{\wp}(\vec{k}\,|\,0;\xi)\Big|_{\vec{k}=0}$. Note that the subscript k here is the number of a dimension of a comb. Not to be confused with the vector $\vec{k}$. From this calculation, the result (24), and the relation

$$\sum_{x_j}e^{ik_jx_j}f_j^{|x_j|}=\frac{1-f_j^2}{1+f_j^2-2f_j\cos k_j}, \tag{25}$$

the authors could obtain the asymptotic behavior of the second moment, for $k\geq 1$,

$$\langle x_k^2\rangle_n\sim\frac{2^{\frac{1}{2^{k-1}}-1}}{\Gamma\left(1+\frac{1}{2^{k-1}}\right)}n^{\frac{1}{2^{k-1}}}. \tag{26}$$

It is obvious that the transport along the primary backbone displays an anomalous diffusion when $k\geq 2$. An anomalous diffusion is a diffusion process with a non-linear

relationship between the mean squared distance from the starting site to the present site and time (the number of steps in this case).

1.2.5 The random walk on Bravais lattices

Since a great deal of problems in solid-state physics are directly or indirectly related to various aspects of random walks on periodic lattices, Montroll and Weiss [24] put their attention on such random walk models. The article of Montroll and Weiss is one of the well-known and most cited articles which are related to the theory of random walks. Because it is a pioneer work that the two crucial concepts of the theory of random walks were first introduced. They include (i) a generic approach often called a generating function formalism (GFF), which was introduced in Subsection 1.2.2, for studying the random walks on finite lattices with periodic boundary conditions and infinite Bravias lattices, and (ii) the extension of the discrete-time random walks, the sparable continuous-time random walks. For sake of simplicity, let us discuss only the discrete-time random walks on infinite Bravais lattices, in particular, cubic lattices.

It is convenient to describe the position of sites $\vec{x}$ on Bravais lattices in Cartesian coordinate, $\vec{x} = x\hat{x} + y\hat{y} + z\hat{z}$. A Bravais lattice is an infinite set of discrete points described in 3-d Euclidean space by equation

$$\vec{x} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 \tag{27}$$

where $\vec{a}_i$ are primitive vectors and n_i are integer numbers. For instance, if the primitive vectors are

$$\begin{gathered}\vec{a}_1 = \hat{x}, \vec{a}_2 = \hat{y}, \vec{a}_3 = \hat{z}, \\ \vec{a}_1 = \hat{y} + \hat{z} - \hat{x}, \vec{a}_2 = \hat{z} + \hat{x} - \hat{y}, \vec{a}_3 = \hat{x} + \hat{y} - \hat{z} \text{ and} \\ \vec{a}_1 = \hat{y} + \hat{z}, \vec{a}_2 = \hat{z} + \hat{x} - \hat{y}, \vec{a}_3 = \hat{x} + \hat{y} - \hat{z},\end{gathered} \tag{28}$$

then the corresponding lattices are respectively called the simple cubic lattice (sc), the body-center cubic lattice (bcc), and the face-center cubic lattice (fcc). The schematics of unit cells of these lattices are shown in Figure 5.

As a random walk is a symmetric Polya walk, the single-step transition probabilities $p(\Delta\vec{x})$ to neighboring sites are equal to the reciprocal of the number of the neighboring sites, i.e.,

$$p(\Delta\vec{x}) = \begin{cases} 1/6 & ;sc \\ 1/8 & ;bcc \\ 1/12 & ;fcc \end{cases} \tag{29}$$

where $\Delta\vec{x}$ is the relative position of neighboring sites to the present site.

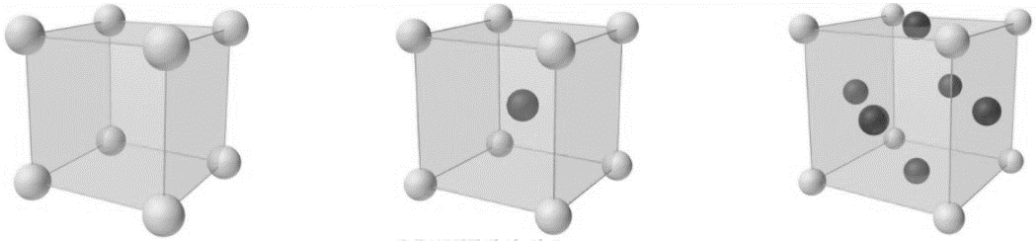


Figure 5. The schematics of unit cells of a simple cubic lattice (left), a body-center cubic lattice (center) and a face-center cubic lattice (right). The dark-colored balls are depicted the lattice sites that are not located at the corners of the unit cells.

From the spatial homogeneity, the probability $\wp(\vec{x})_n$ that a walker is found at a site $\vec{x}$ at the nth step can be described by equation (3), and its Fourier transform of the generating function is

$$\tilde{\wp}(\vec{k};\xi) = \frac{1}{1-\xi\bar{p}(\vec{k})} \tag{30}$$

where $\tilde{\wp}(\vec{k};\xi) \equiv \sum_{\vec{x}} \wp(\vec{x};\xi) e^{\vec{k}\cdot\vec{x}}$ and $\bar{p}(\vec{k}) \equiv \sum_{\Delta\vec{x}} p(\Delta\vec{x}) e^{\vec{k}\cdot\Delta\vec{x}}$. Note that the first sum is over all sites on the structure, but the second sum is only over the neighboring sites. From equations (28) and (29), we have

$$\bar{p}(\vec{k}) = \begin{cases} (c_1+c_2+c_3)/3 & ;sc \\ (c_1c_2+c_2c_3+c_3c_1)/3 & ;bcc \\ c_1c_2c_3 & ;fcc \end{cases} \tag{31}$$

where $c_i = \cos(k_i)$ and $-\pi < k_i \le \pi$.

As mentioned earlier, various random walk properties are encoded in the Fourier transform $\tilde{\wp}(\vec{k};\xi)$. To decode some of them, Montroll and Weiss began with the consideration of the inverse Fourier transform of $\tilde{\wp}(\vec{k};\xi)$ for Bravais lattices in several dimensions,

$$\wp(\vec{x};\xi) = \frac{1}{(2\pi)^k} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \frac{e^{-\vec{k}\cdot\vec{x}}}{1-\xi\bar{p}(\vec{k})} d^k\vec{k}\,, \tag{32}$$

which is the generating function $\wp(\vec{x};\xi) \equiv \sum_{n=0}^{\infty} \wp(\vec{x})_n \xi^n$. Note that the superscript k here is the number of a dimension of the lattice, not the magnitude of the vector $\vec{k}$.

For convenience of further description, let us define the second moment σ_i of each step and the scaling distance squared λ^2 by $\sigma_i \equiv \sum_{\Delta\vec{x}} (\Delta x_i)^2 p(\Delta\vec{x})$ and $\lambda^2 \equiv \sum_{i=1}^{k} \left(\frac{x_i}{\sigma_i}\right)^2$ for $i = 1,...,k$ and $x_1 = x, x_2 = y, x_3 = z$. In addition, let us distinguish the generating functions $\wp(\vec{x};\xi)$ for 1-d, 2-d and 3-d Bravais lattices by the subscript numbers, i.e., $\wp_1(\vec{x};\xi)$, $\wp_2(\vec{x};\xi)$ and $\wp_3(\vec{x};\xi)$, respectively.

The asymptotic expressions of the generating functions $\wp_1(\vec{x};\xi)$ and $\wp_2(\vec{x};\xi)$ were found in the following forms:

$$\wp_1(\vec{x};\xi) \sim \frac{\exp\left(-\lambda\left(2(1-\xi)\right)^{1/2}\right)}{\sigma_1\left(2(1-\xi)\right)^{1/2}}, \tag{33}$$

$$\wp_2(\vec{x};\xi) \sim \frac{1}{\pi\sigma_1\sigma_2} K_0\left(\lambda\left(2(1-\xi)\right)^{1/2}\right), \tag{34}$$

where $K_0(z)$ is a modified Bessel function. In three dimensions and higher, $\wp(\vec{x};\xi)$ is defined by a convergent integral and must be calculated numerically. However, for large λ^2, the asymptotic form of $\wp_3(\vec{x};\xi)$ could be found,

$$\wp_3(\vec{x};\xi) \sim \frac{1}{\pi\sigma_1\sigma_2\sigma_3} \frac{\exp\left(-\lambda\left(2(1-\xi)\right)^{1/2}\right)}{2\lambda}. \tag{35}$$

In various scenarios, these asymptotic forms of the generating functions $\wp(\vec{x};\xi)$ as $\xi \to 1^-$ are sufficient to determine the large time behavior of certain basic random walk properties. The authors employed this fact to treat many basic random walk properties on Bravais lattices. The examples include the mean number $M(\vec{x})_n$ of steps that a site $\vec{x}$ has been visited after n step, and the expected number $\langle S \rangle_n$ of distinct sites visited in an n-step walk.

It was shown that, as $n \to \infty$, $M(\vec{x})_n$ approaches $\lim_{\xi\to 1^-} \wp(\vec{x};\xi)$. Thus, from equations (29) – (35), they could conclude that the mean number of times that any site on 1-d or 2-d Bravais lattices has been visited after large steps is “infinite”. However, for 3-d Bravais lattices, the mean number $M(0)_n$ of steps that the starting site has been visited after many steps is finite, e.g.,

$$M(0)_n = \begin{cases} 1.51639 - 1.31969 n^{-\frac{1}{2}} + \ldots & ; sc \\ 1.39320 - 0.25397 n^{-\frac{1}{2}} + \ldots & ; bcc \\ 1.34466 - 0.46658 n^{-\frac{1}{2}} + \ldots & ; fcc \end{cases}. \quad (36)$$

For the expected number $\langle S \rangle_n$, they found that its generating function $\langle S \rangle(\xi)$ has a simple relation to the generating function $\wp(0;\xi)$ of the probability of return to the starting site,

$$\langle S \rangle(\xi) = \frac{1}{(1-\xi)^2 \wp(0;\xi)}. \quad (37)$$

Therefore, from this relation, equations (29) – (35) and the Tauberian theorem for discrete power series method (see, e.g., [1]), if we choose $\sigma_1 = 0.5$, $\sigma_1\sigma_2 = 1$ and $\sigma_1\sigma_2\sigma_3 = 1$, we will obtain the asymptotic forms of the expected number $\langle S \rangle_n$ as

$$\langle S \rangle_n \sim \begin{cases} (8n/\pi)^{\frac{1}{2}} & ;1\text{-d} \\ \pi n/\log n & ;2\text{-d} \\ n/\lim_{\xi \to 1^-} \wp(0;\xi) & ;3\text{-d} \end{cases}. \quad (38)$$

1.2.6 The random walk on Bethe lattices

Hughes and Sahimi extended GFF for random walks on Bravais lattices to Bethe lattices [37]. Bethe lattice is a loopless structure or the so-called tree-like structure such that (i) each site has $z \geq 2$ neighboring sites, and (ii) there are no closed loops. The structure of the Bethe lattice with $z = 3$ is partially shown in Figure 6. As you can imagine, Bethe lattices cannot be embedded comfortably in finite-dimensional Euclidean spaces, so they are often called pseudo-lattices.

From the topological equivalence of all sites, any site of Bethe lattices can be chosen as origin of coordinates. Furthermore, since Bethe lattices are loopless structures, the chosen origin is connected to a given site by a unique path. The coordinate of that site can be assigned by the number x of edges making up the path from the given site to the origin. Accordingly, there are z sites with $x = 1$, and there are in general $z(z-1)^{x-1}$ sites with the same coordinate $x > 1$.

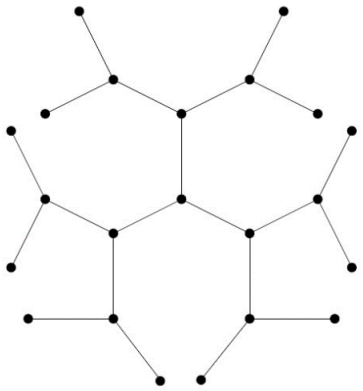


Figure 6. A piece of the Bethe lattice with $z=3$.

The authors restricted themselves to the symmetric Polya walk. They noticed that steps will either take the walker further from the origin with probability $(z-1)/z$, or closer to the origin with probability $1/z$. The walker can therefore be described as the asymmetric random walk on a restricted 1-d lattice. The conditional probability $\wp(x\,|\,x_0)_n$ that a walker has coordinate x after n steps, given that the walker initiated at coordinate x_0, obeys the recursive relation

$$\wp(x\,|\,x_0)_n=\delta_{n,0}\delta_{x,x_0}+\sum_{x'}p(x,x')\wp(x'\,|\,x_0)_{n-1} \tag{39}$$

with the single-step transition probability $p(x,x')$ depending on the past coordinate,

$$p(x,x')=\begin{cases}\dfrac{z-1}{z}\delta_{x,x'+1}+\dfrac{1}{z}\delta_{x,x'-1} & ;x'\geq 1\\ \delta_{x,x'+1} & ;x'=0\end{cases}. \tag{40}$$

In this setup, the authors could express the explicit form of the generating function $\wp(x;\xi\,|\,x_0)$, whose the expression is too complicated to be expressed here. The generating function led to many basic random walk properties on Bethe lattices. For instance, the probability of ever reaching the sites with coordinate x, given that the walker initiated at the origin, is

$$R(x)=\begin{cases}1/(z-1) & ;x=0\\ (z-1)^{-x} & ;x\geq 1\end{cases}. \tag{41}$$

It should be noted that, only $z=2$, every site on the structure is eventually reached by the walker. The conditional mean first-passage time $\tau(x)$ to the sites with

coordinate x, given that the walker initiated at the origin and eventually reaches those sites, was also obtained,

$$\tau(x)=\begin{cases}2(z-1)/(z-2) & ;x=0\\ xz/(z-2) & ;x\geq 1\end{cases}. \tag{42}$$

It should also be remarked that the conditional mean first-passage time $\tau(x)$ is infinite for every site on the structure when $z=2$, otherwise it is finite. The final instance is the expected number $\langle S\rangle_n$ of distinct sites visited after n steps,

$$\langle S\rangle_n \sim \begin{cases}(8n/\pi)^{\frac{1}{2}} & ;z=2\\ \dfrac{(z-2)}{(z-1)}n & ;z>2\end{cases}. \tag{43}$$

1.2.7 The random walk on intersecting geometries

One of more recent studies of a random walk on peculiar structures by GFF is the work of Sepehrinia, Saberi and Dashti-Naserabadi [8]. They presented the discrete-time random walk on the geometry composed of an infinite lattice plane $\mathbb{Z}^2$ which is crossed by the n_l numbers of lattice lines $\mathbb{Z}$ that they share a single common site – the origin.

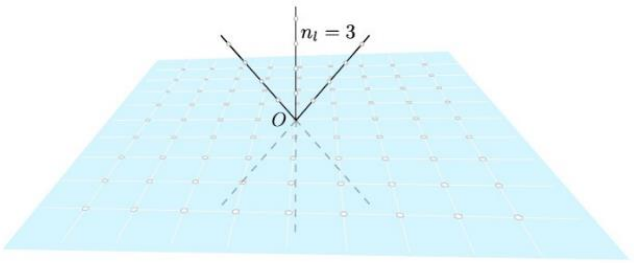


Figure 7. An illustration of the mixed geometry consisting of an infinite lattice plane $\mathbb{Z}^2$ which is crossed by the three lattice lines $\mathbb{Z}$ [8].

Their starting point was the consideration of a general case that two general lattices a and b, on which the random walk problem is known. The lattices are connected to each other in a way that they have a single point in common which is called the origin O. In addition, it is assumed that a walk is Polya walk and starts at the origin O. Depending on the geometry of the two lattices which share a single

common site O, the authors noticed that the first-passage probability $\mathcal{F}(0)_n$ of return to the origin O can be decomposed into two terms,

$$\mathcal{F}(0)_n = p_a \mathcal{F}_a(0)_n + p_b \mathcal{F}_b(0)_n \tag{44}$$

where $p_a + p_b = 1$. The first term is the first-passage probability $\mathcal{F}_a(0)_n$ of return to the origin for isolated lattice a timed the probability p_a that, at the first step, the walker would enter into the lattice a. The second term is analogous to the first term. The authors employed the idea analogous to the relation (21) to relate the first-passage probability $\mathcal{F}(0)_n$ to the probability $\wp(0)_n$ that the walker is found at the origin O,

$$\wp(0)_n = \delta_{0,n} + \sum_{n'=0}^{n} \wp(0)_{n'} \mathcal{F}(0)_{n-n'}. \tag{45}$$

For $\vec{x} \neq 0$, the probability $\wp(\vec{x})_n$ that the walker is found at a site $\vec{x}$ can be considered as the sum of the probability of being at the origin at any earlier step $n' < n$ and arriving to the destination without visiting the origin on the remaining step $n - n'$. In other words,

$$\wp(\vec{x})_n = \sum_{n'=0}^{n-1} \wp(0)_{n'} T(\vec{x})_{n-n'} \tag{46}$$

where $T(\vec{x})_n$ is the probability that the walker arrives at the destination $\vec{x}$ without visiting the origin on the time n.

From the relations (44) – (46), the authors could derive the generating functions $\wp(\vec{x};\xi)$ of the probabilities $\wp(\vec{x})_n$ in terms of the generating functions in the individual geometries, for $\vec{x} = 0$,

$$\frac{1}{\wp(0;\xi)} = \frac{p_a}{\wp_a(0;\xi)} + \frac{p_b}{\wp_b(0;\xi)}, \tag{47}$$

and, for $\vec{x} \neq 0$,

$$\wp(\vec{x};\xi) = \wp(0;\xi) \times \begin{cases} p_a T_a(\vec{x};\xi) \\ p_b T_b(\vec{x};\xi) \end{cases}. \tag{48}$$

For a translationally invariant lattice, it can be shown that, for $\vec{x} \neq O$,

$$T_{a,b}(\vec{x};\xi) = \frac{\wp_{a,b}(\vec{x};\xi)}{\wp_{a,b}(0;\xi)}. \tag{49}$$

For taking a to be an infinite lattice plane $\mathbb{Z}^2$ and b to be the n_l numbers of lattice lines $\mathbb{Z}$, they found that the probability $\wp(0)_n$ of return to the starting site

O after n steps behaves differently in two different time regimes which are separated by a crossover time n_c. This crossover time is approximately proportional to the numbers of lattice lines squared, $n_c \propto n_l^2$. When $n \ll n_c$, the line geometry governs the behavior of the random walk and $\wp(0)_n \propto n^{-1/2}$. While $n \gg n_c$, the plane geometry governs the behavior $\wp(0)_n \propto n^{-1}$. Moreover, they also showed the different asymptotic behavior of the mean-squared distance of the random walk location on the plane and on crossing lattice lines, which are defined by $\langle x_p^2 \rangle_n \equiv \sum_{\vec{x} \in p} |\vec{x}|^2 \wp(\vec{x})_n$ and $\langle x_l^2 \rangle_n \equiv \sum_{\vec{x} \in l} |\vec{x}|^2 \wp(\vec{x})_n$ respectively,

$$\langle x_p^2 \rangle_n \sim n, \tag{50}$$

$$\langle x_l^2 \rangle_n \sim \sqrt{2/\pi^3}\, n_l \sqrt{n} \log(n). \tag{51}$$

1.2.8 The random walk on restricted 1-d lattices

Before ending this subsection, let us discuss one of basic models of theory of random walks, a discrete-time random walk on 1-d finite lattices, i.e., the set of integers $S = \{0,1,...,N\}$, with asymmetric imperfect absorbing barriers at the ending sites. A walker, initiating at $x_0 \in S$, takes a step to the right or the left neighboring sites with probabilities p and q, respectively. In addition, it possibly does not take any step with probability $r = 1-(p+q)$ for $0 \le p,q \le 1$. If the ending sites 0 or N are reached, the walker may be absorbed or reflected with respective probabilities $1-\rho$ and ρ at 0 and $1-\omega$ and ω at N, for $0 \le \rho,\omega \le 1$. A schematic illustration of this model is shown in the following figure.

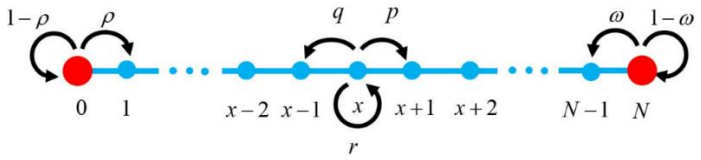


Figure 8. A schematic illustration of a trinomial random walk on a 1-d finite lattice with two imperfect absorbing barriers.

Such models are the generalization of many particular random walk problems, for instance, the classical ruin problem (see, e.g., Feller (1968) [38]). We

discuss this basic model at this last subsection not because it is unimportant, but because it is important, and its results will often be referred latter.

Let $\wp\left(x\,|\,x_0\right)_n$ be the probability that a walker is found at a site x at the n th step, given that it initiated at a site x_0, for $x, x_0 \in S$. Then $\wp\left(x\,|\,x_0\right)_n$ satisfies the following recursive equation: For $n \geq 1,\ x \in \{2,3,...,N-2\}$,

$$\wp\left(x\,|\,x_0\right)_n = q\wp\left(x+1\,|\,x_0\right)_{n-1} + r\wp\left(x\,|\,x_0\right)_{n-1} + p\wp\left(x-1\,|\,x_0\right)_{n-1}. \tag{52}$$

Subject to the following "initial and boundary" conditions:

$$\wp\left(x\,|\,x_0\right)_0 = \delta_{x,x_0},\ \wp\left(0\,|\,x_0\right)_n = q\wp\left(1\,|\,x_0\right)_{n-1},\ \wp\left(N\,|\,x_0\right)_n = p\wp\left(N-1\,|\,x_0\right)_{n-1},$$
$$\wp\left(1\,|\,x_0\right)_n = \rho\wp\left(0\,|\,x_0\right)_{n-1} + r\wp\left(1\,|\,x_0\right)_{n-1} + q\wp\left(2\,|\,x_0\right)_{n-1} \text{ and}$$
$$\wp\left(N-1\,|\,x_0\right)_n = p\wp\left(N-2\,|\,x_0\right)_{n-1} + r\wp\left(N-1\,|\,x_0\right)_{n-1} + \omega\wp\left(N\,|\,x_0\right)_{n-1}.$$

El-Shehawey [39] found the closed form of the generating function $\wp\left(x;\xi\,|\,x_0\right) \equiv \sum_{n=0}^{\infty} \wp\left(x\,|\,x_0\right)_n \xi^n$ for $x, x_0 \in S$, but unfortunately, it cannot be expressed in a trivial form. For the sake of clarity and simplicity, let us consider only two special cases including binomial random walks, $r = 0$, on the 1-d finite lattice with two perfect absorbing sites, i.e., $\rho, \omega = 0$, and on the 1-d finite lattice with one perfect absorbing site and one perfect reflecting site, i.e., $\rho = 0$ and $\omega = 1$. In addition, we direct our attention to the generating functions of the absorbing probability, i.e., $\wp\left(x;\xi\,|\,x_0\right)$ where the site x is only an absorbing point.

It is noteworthy to mention that when the expression of the generating function $\wp\left(x;\xi\,|\,x_0\right)$ is known, we can calculate the mean step or the mean time τ that the walker spends before arriving at the site x from the limit of the derivative of the generating function, i.e., $\tau = \lim_{\xi \to 1^-} \frac{\partial}{\partial \xi} \wp\left(x;\xi\,|\,x_0\right)$.

Since the special cases are considered, let us introduce new notations for the corresponding generating functions. Let $U^{(H)}\left(p, N;\xi|x_0\right)$ denote the generating function of the probability that a walker on the lattice with two perfect absorbing sites, in which the walker initiated at a site $x_0 \in \{1,2,3,...,N-1\}$ and it is biased to the right neighboring site with probability p, is absorbed at the absorbing sites N. From the finding results of El-Shehawey, the generating function $U^{(H)}\left(p, N;\xi|x_0\right)$ can be expressed in the following form:

$$U^{(H)}\left(p,N;\xi\middle|x_0\right)=\frac{\lambda_+^{x_0}\left(p;\xi\right)-\lambda_-^{x_0}\left(p;\xi\right)}{\lambda_+^{N}\left(p;\xi\right)-\lambda_-^{N}\left(p;\xi\right)} \tag{53}$$

where $\lambda_\pm\left(p;\xi\right)=\frac{1\pm\sqrt{1-4p\left(1-p\right)\xi^2}}{2p\xi}$. Note that the limit $\lim_{\xi\to1^-}U^{(H)}\left(p,N;\xi\middle|x_0\right)$ is the probability that the walker is absorbed at N on regardless of the number of steps.

According to the above-mentioned note, from this resulting generating function, we can furthermore obtain the mean absorbing time from $\tau^{(H)}\left(p,N\middle|x_0\right)=\lim_{\xi\to1^-}\frac{\partial}{\partial\xi}U^{(H)}\left(p,N;\xi\middle|x_0\right)$. For later analysis, the mean absorbing time for the initial sites next to the absorbing sites are required,

$$\tau^{(H)}\left(p,N\middle|1\right)=\frac{\left(a+1\right)-\frac{N\left(a^N+1\right)\left(a-1\right)}{\left(a^N-1\right)}}{\left(2p-1\right)\left(a^N-1\right)}, \tag{54}$$

$$\tau^{(H)}\left(p,N\middle|N-1\right)=\frac{\left(N-1\right)\left(a^{N-1}+1\right)-\frac{N\left(a^N+1\right)\left(a^{N-1}-1\right)}{\left(a^N-1\right)}}{\left(2p-1\right)\left(a^N-1\right)} \tag{55}$$

where $a\equiv\left(1-p\right)/p$. Regardless of at which absorbing site the walker is absorbed, the mean absorbing time can be calculated from the sum

$$\tau^{(H)}\left(p,x_0\right)\equiv\tau^{(H)}\left(p,N\middle|x_0\right)+\tau^{(H)}\left(1-p,N\middle|N-x_0\right). \tag{56}$$

Therefore, for the initial sites $x_0=1$ and $x_0=N-1$, we have

$$\tau_\alpha\left(p,N\right)\equiv\tau^{(H)}\left(p\middle|1\right)=\frac{1}{1-2p}\left(1-N\left(\frac{1-a}{1-a^N}\right)\right), \tag{57}$$

$$\tau_\gamma\left(p,N\right)\equiv\tau^{(H)}\left(p\middle|N-1\right)=\frac{1}{1-2p}\left(\left(N-1\right)-N\left(\frac{1-a^{N-1}}{1-a^N}\right)\right). \tag{58}$$

The new notations introduced here will make sense to you later.

Analogously, let $U^{(V)}\left(p,N;\xi\right)$ denote the generating function of the probability that a random walker on the lattice with one perfect absorbing site and one perfect reflecting site, which the walker initiated at the site $x_0=1$ and it is biased to the right neighboring site with probability p, is absorbed at the absorbing site 0. On one hand, for finite-length lattices, $N<\infty$, it can be shown that

$$U^{(V)}\left(p,N;\xi\right)=\left(\frac{1-p}{p}\right)\frac{u\left(p,N,1;\xi\right)}{u\left(p,N,0;\xi\right)} \tag{59}$$

where $u(p,N,j;\xi)\equiv\left(\lambda_+^{N-j}(p;\xi)-\lambda_-^{N-j}(p;\xi)\right)-\xi\left(\lambda_+^{N-j-1}(p;\xi)-\lambda_-^{N-j-1}(p;\xi)\right)$.
The corresponding mean absorbing time denoted by $\tau_\beta(p,N)$ is

$$\tau_\beta(p,N)=\frac{1}{1-2p}\left(1-\frac{2(1-p)}{a^N}\right). \tag{60}$$

On the other hand, if the length of lattice is infinite, then the generating function becomes

$$U^{(V)}(p,\infty;\xi)=\lambda_-(p;\xi). \tag{61}$$

Again, note that the limit $\lim_{\xi\to 1^-}U^{(V)}(p,\infty;\xi)$ is the probability that the walker is absorbed, regardless of the number of steps. From equation (61), we have

$$\lim_{\xi\to 1^-}U^{(V)}(p,\infty;\xi)=\begin{cases}1 & p\le 0.5\\ 1/p-1 & p>0.5\end{cases}. \tag{62}$$

This result confirms our intuition. When the walker is unbiased or biased towards to the absorbing site, the event that the walker is absorbed is certain to happen. Otherwise, the probability of the event is less than unity. For $p=0.5$, the mean absorbing time is infinite, but, for $p<0.5$, it is finite,

$$\tau_\beta(p,\infty)=\frac{1}{1-2p}. \tag{63}$$

From what have been presented so far, we should be convinced that the problems of random walks on structures of different topologies are still open and challenging. Among various structures, the so-called quasi-1d structures have also attracted very wide interests because they are ubiquitous and possess remarkable properties. Examples include macromolecules, e.g., polymers and deoxyribonucleic acids (DNAs) and artificial materials, e.g., carbon nanotubes and nanowires. If the length of this kind of materials is considerably large, then the end effects can be neglected and the length of the materials can be assumed infinite. A number of problems relevant to such materials are directly or indirectly related to various aspects of random walks on quasi-1d infinite structures, which is the subject of this thesis. Before embarking on a detailed mathematical theory, it may be useful to have in mind a picture of how the concept of the random walks on quasi-1d infinite structures is feasibly related to the study of quasi-1d materials. Therefore, in the following section, a survey of these relations will be given.

1.3 Quasi-1d materials

1.3.1 Spiny dendrites

A dendrite is a branched protoplasmic extension of a nerve cell that propagates input received from other cells to the cell body of the neuron. There are two types of dendrites including smooth dendrites and spiny dendrites (see Figure 9). A spiny dendrite is a dendrite with small protrusions or the so-called spines, which are composed of a head and a thin neck located on the surface of dendrites. These spines are thought to be key elements in neuronal information processing. Decreasing spine density can result in cognitive disorders, such as autism, mental retardation and fragile X syndrome.

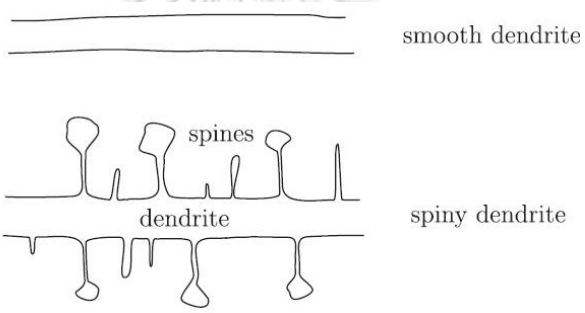


Figure 9. A schematic drawing of smooth and spiny dendrites [6].

Experiments together with numerical simulations have shown that the transport of inert particles along the axis of smooth dendrite is normal diffusive, the mean square distance along the axis grows linearly with times. On the other hand, the diffusion over spiny dendrite is anomalous diffusive.

Mendez and Iomin [6] suggested a random walk on comb-like structures to describe this anomalous transport in spiny dendrites. Geometry of the comb structure makes it possible to describe anomalous diffusion, where branches and the backbone correspond to spines and the dendritic axis respectively. They found that the anomalous diffusion along the dendritic axis is controlled by the fractal geometry of the comb structure and the fractional kinetics inside the spines.

1.3.2 Polymers

Polymers are long chains composed of many repeating subunits known as monomers. The properties of the monomers thus determine unique physical properties of the polymer, e.g., toughness, elasticity, viscoelasticity, and tendency to form amorphous and semicrystalline structures rather than crystals. For instance, schizophyllan is a triple-helical polymer whose monomers are β-1,3-glucan with one side chain glucose residue. The structure of schizophyllan and the chemical structure of the monomer are schematically shown in Figure 10.

From the study of dielectric relaxation in aqueous solutions of schizophyllan [40], it was shown that, because of the unique conformation of this kind of polymers, it induces an ordered structure about the helix core, which consists of the side-chain glucose residue and nearby water molecules.

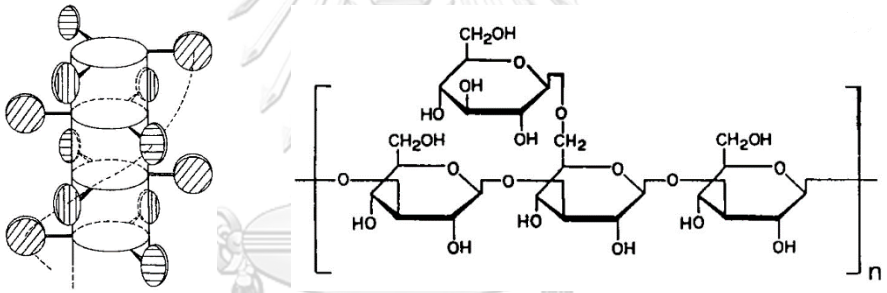


Figure 10. A schematic of the structure of schizophyllan (left) and the chemical structure of the monomer (right) [40].

As we know, a relaxation measurement is reliable method to probe many properties of the aqueous polymer solutions. In wide range of the relaxation processes, they have been implicated in the stretch exponential decay profiles [41],

$$\varphi(t) = \exp\left(-\left(\frac{t}{\tau_H}\right)^{\beta}\right) \tag{64}$$

where $\varphi(t)$ is denoted as the relaxation function, τ_H is the relaxation time of the process and $0 < \beta \leq 1$. Several authors have proposed mesoscopic models describing these stretched exponential relaxations. One of the interesting models is the defect-diffusion model based on random walk models [42].

There are numerous relaxation phenomena involving to polymeric systems. For sake of simplicity, let us discuss the relaxation of the average $R(t)$ of the end-to-end distance of polymers in a solution [43, 44]. In the language of the defect-diffusion model, it is assumed that there is a large number of non-interacting defects, e.g., kinks, diffusing on a polymer, which is assumed to be a 1-d lattice. The average $R(t)$ returns to equilibrium from an initially perturbed state when at least one defect leaves the chain. This is directly related to the problem of the first-passage time of a random walk on a 1-d lattice. Altogether, in certain limits, it can be shown that the relaxation function obeys the stretch exponential function. In addition, Bendler and Shlasinger [42] qualitatively proposed that the relaxation time τ_H of this process is proportional to a power function of the number M of the monomers,

$$\tau_H \propto M^{1/\beta} \tag{65}$$

where β is the same exponent in equation (64).

1.3.3 Deoxyribonucleic acids

A deoxyribonucleic acid (DNA) is a macromolecule composed of two polynucleotide chains that coil around each other to form a double helix. DNAs carry genetic instruction for many biological processes, e.g., the development, functioning, growth and reproduction of all known organisms and many viruses. The phenomenon of specific molecular recognition between a DNA-binding protein and its specific target DNA sequence lies at the heart of these processes. Clearly, timing is critical for the recognition events. A failure to rapidly find the target DNA sequence possibly results in cellular malfunction, because the recognition events are often part of a cascade of various essential events.

It has been shown that the protein recognizes its DNA target through a combination of “one-dimensional” diffusion, the protein “slides” or “hops” along the DNA, and “three-dimensional” diffusion, the protein may move away from the DNA and diffuse into 3D bulk. The search time is determined by the partitioning between these two diffusion modes. Krepel and Levy [45] numerically studied the effect of the crowded environment, a mixture of particles with entropic and energetic effects, on this partitioning. An illustration of this DNA searching of a protein

in the presence of crowding particles is shown in Figure 11. Their main findings are that adding crowders with affinity to the DNA reduces the efficiency of crowding as a searching facilitator that increases one-dimensional diffusion, and therefore increases the mean of the searching time.

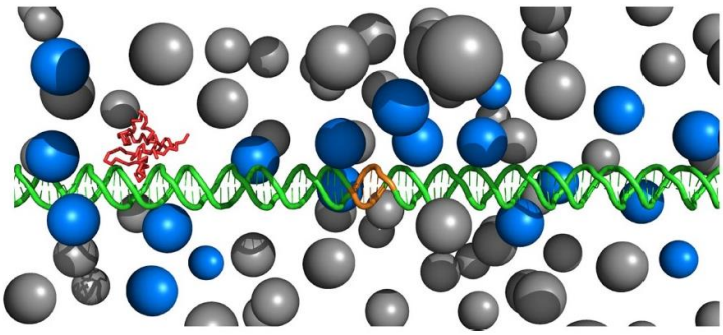


Figure 11. An illustration of recognition by a protein (red) of its DNA (green) target site (orange) [45].

From a resemblance of the random motion of a protein with two-mode diffusions in the vicinity of a DNA and a 2-state random walk on a 1-d lattice, the problem of the DNA searching by a protein in the presence of crowding particles may be transcribed into the random walk language (see Section 5.5). Therefore, one may employ the manipulations developed under the random walk framework to investigate properties of interest in the problem of the DNA searching. For instance, the mean of the searching time may be evaluated from the mean first-passage time.

1.3.4 Carbon nanotubes

A carbon nanotube is a hollow cylindrical lattice made of carbons with diameter measured in nanometers. They often refer to single-wall carbon nanotubes. In convention, they are classified by treating how they are formed by rolling up graphene sheets as shown in Figure 12.

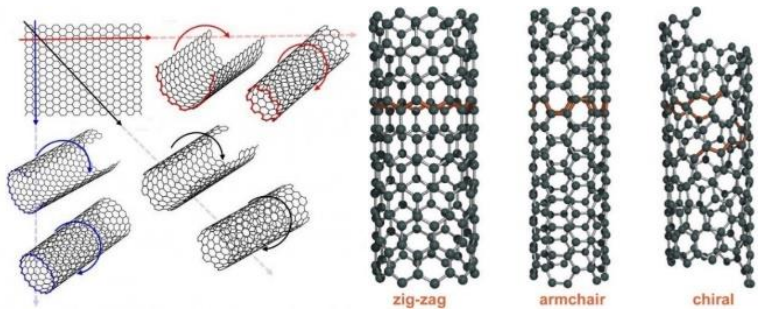


Figure 12. The structures of three kinds of the single-wall carbon nanotubes [46].

Carbon nanotubes have drawn attention from many authors due to a certain number of remarkable properties, which lead to a new carbon nanotube-based technology. Recent investigations have focused on the carbon nanotube-based Lithium (Li) ion batteries. The development of the efficiency of the batteries, i.e., charge and discharge rate, capacity, and cyclability, relies on the understanding of the diffusion and the intercalation of Li ions in carbon nanotubes.

An example study is the work of Song, Yang, Zhao and Fang [47]. They numerically studied the diffusion and the intercalation of Li ions in a carbon nanotube bundle. They found that lithium ions quickly penetrate into the carbon nanotubes and the space between the neighboring carbon nanotubes, and they tend to remain in those spaces. If the density of Li ions is low, they prefer to be close to the carbon nanotube ends. When the density of Li ions is greatly increased, the ions stay either inside the nanotubes or in the interstitial space between neighboring nanotubes.

Just as a suggestion, according to the feasibility of ion intercalation and its reversion through appropriate electrical actions, e.g., the combination of electrons and ions, the point view of the electron hopping on a carbon nanotube from variable range hopping mechanism [48] together with the concept of random walks on hollow cylindrical lattice may be used to investigate the rate of the intercalation or its reversion, which dominates more or less the charge and the discharge rate of the batteries.

1.3.5 Nanowires

According to the lack of efficient methods to fabricate carbon nanotubes with specific electrical characteristics, some authors have directed their attention to the study of nanowires, nanostructures with the diameters of the order of nanometers. In the current trend of device miniaturization, these quasi-1d nanostructures play a significant role as the building blocks for devices that could overcome the fundamental limits of microtechnology. Figure 13. shows (a) SEM image of Nb_2PdS_5 single-crystal nanowires with different cross-sectional areas, and (b) crystallographic structure of Nb_2PdS_5 with 1d chains along b-axis.

One of fundamental problems in electronic transport study of nanowires is to deduce the dependence of current on bias voltage. Interestingly, at low temperature, a great number of nanowires, e.g., semiconductor nanowires [49], MoSe nanowires [50], $NbSe_3$ nanowires [51] and gold nanowires [52], behaves as a non-ohmic resistor. In other words, the power-law dependence of current on bias voltage, $I \propto V^{1+\eta}$, has been observed. The "anomalous" exponent η is rooted on the quasi-1d confinement and the existence of defects or disorders.

Although many authors have studied on transport properties of nanowires, they have not encountered any investigation of basic statistical properties of random walks on such structures, which may reveal some insights of transport in nanowires (see Section 6.3).

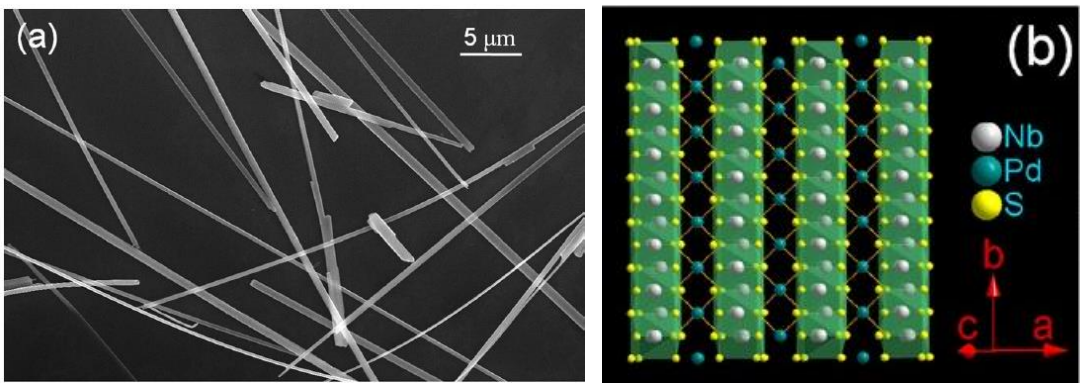


Figure 13. (a) SEM image of Nb_2PdS_5 single-crystal nanowires, and (b) crystallographic structure of Nb_2PdS_5 [53].

1.4 Our work

In this thesis, we consider a separable continuous-time random walk on quasi-1d lattices as a model for transport processes on quasi-1d materials. A quasi-1d lattice consists of periodically repeated unit cells with the following properties: In the unit cell, (i) there exists particular sites named “major” sites, which are connected to their equivalent sites in neighboring unit cells by a certain kind of network; and (ii) there may be dangling networks attached to the major sites.

The thesis is divided into two parts. In the first part (Chapter 2), the model is clarified in more details (Section 2.1) following with the development of a general formalism (Section 2.2). We exploit the fact, that if a walker with nearest-neighboring steps is at a certain site on the quasi-1d lattices, it must be at the major sites, which are located in the present unit cell or the neighboring unit cells, at some earlier steps, to formulate the recursive equation of the probability that the walker is found at a given site at a certain step, i.e., Chapman- Kolmogorov equation. More precisely, the probability to arrive at a given site at a certain step can be considered as the sum of the multiplication of the probabilities of being at the major sites, which are located in the present unit cell or the neighboring unit cells, at any earlier step and the multi-step transition probabilities to the destination without visiting any major sites on the remaining steps. In addition, we assume that, between jumps, a walker waits for a random time, distributed according to a general probability distribution function.

Since the random motion of the walker can be described by the recursive equation, we will develop a formalism based on GFF together with the concept of irreducible Markov chains. The resulting formalism paves the way for formulating a method that allows us to asymptotically describe some basic statistical properties of the random walks.

In general, for large times, basic dynamical random walk properties are characterized by certain prefactors and time exponents, which reflect the localized transport of a walker and the geometrical characteristics of the underlying structure. The main goal of this thesis is to develop a systematic method to calculate the values of these parameters (Section 2.3).

In the second part of the thesis (Chapter 3 - 6), the applications of the developed method to certain concrete models are demonstrated. We begin with the simplest model, the random walk on an unrestricted 1-d lattice served as comparison of the later analysis. Then we consider the random walk on branched lattices which the 2-d comb structure is their special case. Afterward, more complex models are investigated including the random walk on ladder lattices which may be related in some way to the problems of the 2-state particle on a 1-d lattice, and the random walk on cylindrical lattices which can be thought as caricatures of natural and artificial structures, e.g., carbon nanotubes.

A journey of thoughts starts here.

2

Model and general formalism

2.1 Model

We consider a separable continuous-time random walk (SCTRW) on quasi-1d lattices as a model for transport processes on quasi-1d materials. The random walk process, first introduced by Montroll and Weiss [24], is separable in a sense that the probabilities of the waiting time and of the jumping step are independent. We will assume that all walks are Polya walks, walks in which steps to neighboring sites only are allowed. On the other hand, a quasi-1d lattice is defined as a lattice system consists of periodically repeated unit cells connecting to each other in a one-dimensional fashion. A schematic of this kind of structures is shown below.

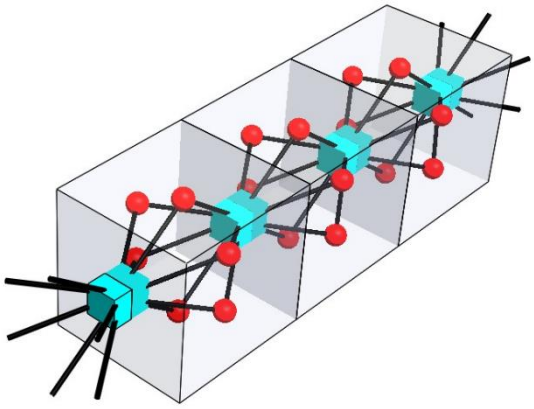


Figure 14. A schematic of the structure of the quasi-1d lattices. The unit cell contains major sites (red spheres) and connected lattice networks (blue boxes).

In each unit cell, there exists different N_M sites (red spheres) which are connected to their equivalent sites in the next unit cell by a certain lattice network (a blue box). For ease of reference, let us call these sites “major” sites and the

others “minor” sites. Each major site may be attached with a dangling lattice network, which is not explicitly shown in Figure 14. The line passing through a certain set of equivalent major sites is called the “structure axis”. It is assumed that the connected lattice networks consist of $N - N_M$ different minor sites. Thus, each unit cell contains N different sites. The following figure shows some concrete examples of the quasi-1d lattices.

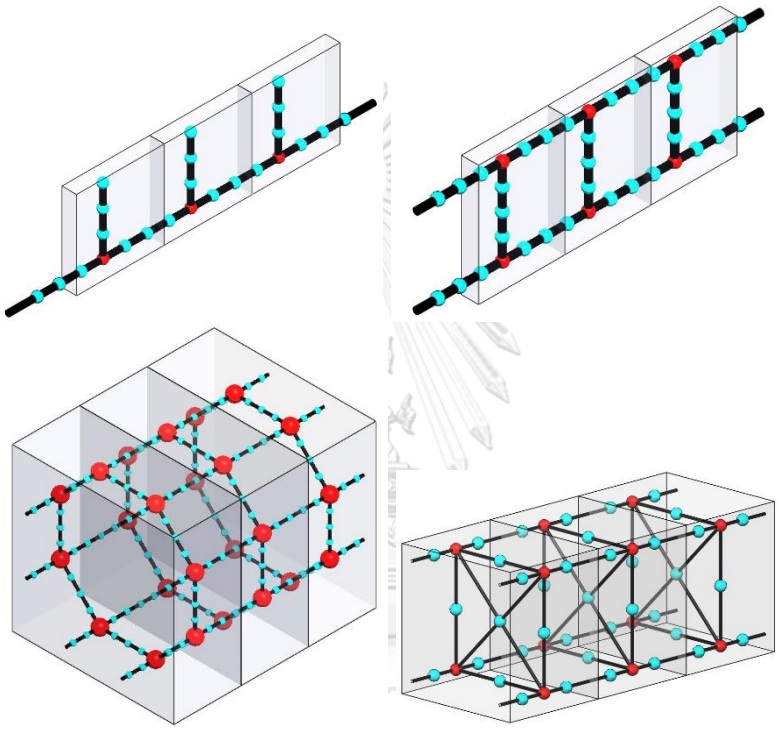


Figure 15. Unit cells of the several concrete examples of the quasi-1d infinite structures.

To indicate position of a site on such structures, the Cartesian coordinate system (x, y, z) defined such that the x axis coincides with the structure axis is used and the distance between neighboring sites is unity for simplicity. With this coordinate system, a fundamental translation vector is given by $L\hat{x}$ where $\hat{x}$ is a unit vector and L is the linear size of a unit cell along the structure axis. The origin O is placed at a certain major site on the structure axis within a unit cell, labelled the 0 th unit cell. Unit cells and sites within each unit cell are labelled respectively by letters m and a. The position of the major site equivalent to the origin O within

the m th unit cell is thus given by $mL\hat{x}$. The relative positions of sites within the unit cell to this major site are denoted by $\vec{r}_1, \vec{r}_2, \vec{r}_3, ..., \vec{r}_N$ where the vector $\vec{r}_1 = 0$ is for this major site itself, the vectors $\vec{r}_2, \vec{r}_3, ..., \vec{r}_{N_M}$ are for the remaining major sites and the vectors $\vec{r}_{N_M+1}, \vec{r}_{N_M+2}, \vec{r}_{N_M+3}, ..., \vec{r}_N$ are for the minor sites. Accordingly, the position of the a site in the m th unit cell indicated by the vector $\vec{x}_{m,a}$ may be represented as $\vec{x}_{m,a} \equiv mL\hat{x} + \vec{r}_a$ where $a = 1, 2, 3, ..., N$ or the 3-tuple $\left(x_{m,a}, y_{m,a}, z_{m,a}\right)$. Figure 16 illustrates the arrows representing certain elementary vectors of the structure in Figure 14.

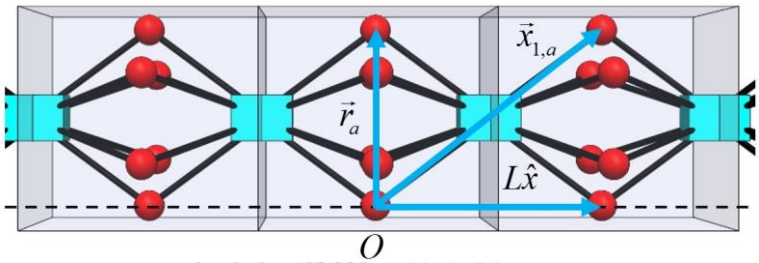


Figure 16. The side view of the 0 th unit cell and its neighboring unit cells of the structure in Figure 14. The dash line and the blue arrows represent the structure axis and certain vectors, respectively.

2.2 General formalism

Let $\wp\left(\vec{x}_{m,a} \mid \vec{x}_{0,b}\right)_n$ be the conditional probability that a walker takes the n th step to a site $\vec{x}_{m,a}$, given that the starting site is a major site $\vec{x}_{0,b}$, and $\psi(t)_n\, dt$ be the probability that the walker takes the n th step at time t. Altogether, the conditional probability that the walker takes the n th step to the site $\vec{x}_{m,a}$ at time t can thus be written as

$$\wp\left(\vec{x}_{m,a} \mid \vec{x}_{0,b}\right)_n \psi(t)_n\, dt. \tag{66}$$

It is assumed that $\psi(t)_n$ obeys the recursive relation

$$\psi(t)_n = \int_0^t \psi(t-t')_{n-1} \psi(t')\, dt' \tag{67}$$

and $\psi(t)_0 = \delta(t)$, where $\psi(t)$ is the probability distribution function (PDF) of waiting time of between two steps. As the walker starts from the major site $\vec{x}_{0,b}$, we have

$$\wp\left(\vec{x}_{m,a} \mid \vec{x}_{0,b}\right)_0 = \delta_{m,0}\delta_{a,b}\,. \tag{68}$$

We can therefore find that the conditional probability $\wp\left(\vec{x}_{m,a}, t \mid \vec{x}_{0,b}\right)$ of the walker being found at the site $\vec{x}_{m,a}$ at time t can be expressed as

$$\wp\left(\vec{x}_{m,a}, t \mid \vec{x}_{0,b}\right) = \int_0^t \left(\sum_{n=0}^{\infty} \wp\left(\vec{x}_{m,a} \mid \vec{x}_{0,b}\right)_n \psi\left(t'\right)_n \right) \Psi\left(t - t'\right) dt' \tag{69}$$

where $\Psi\left(t\right) \equiv \int_t^{\infty} \psi\left(t'\right) dt'$ is the so-called survival probability on a site, the probability that the waiting time on a site exceeds t. In words, the conditional probability $\wp\left(\vec{x}_{m,a}, t \mid \vec{x}_{0,b}\right)$ can be considered as the sum of the probabilities of the walker transition to the site $\vec{x}_{m,a}$ at different steps and times, provided the waiting time on that site exceeding $t - t'$ after its arrival to the site $\vec{x}_{m,a}$ at time t'.

Note on notations, unless otherwise stated, we will hereafter use the following definitions of Fourier transform in mL and Laplace transform in t,

$$f\left(\vec{x}_{m,a}\right) \overset{F}{\rightarrow} \tilde{f}\left(k, \vec{r}_a\right) \equiv \sum_{m=-\infty}^{\infty} f\left(\vec{x}_{m,a}\right) e^{ikmL}\,, \tag{70}$$

$$f\left(t\right) \overset{L}{\rightarrow} f^*\left(s\right) \equiv \int_0^{\infty} f\left(t\right) e^{-st} dt\,, \tag{71}$$

and a generating function,

$$f\left(\cdot\right)_n \overset{G}{\rightarrow} f\left(\cdot;\xi\right) \equiv \sum_{n=0}^{\infty} f\left(\cdot\right)_n \xi^n\,, \tag{72}$$

where $-\pi/L < k \le \pi/L$, $s > 0$, $-1 < \xi < 1$ and assume that they exist. Furthermore, to distinguish the probabilities for major sites from the probabilities for general sites, we define

$$P_{ab}\left(m\right)_n \equiv \wp\left(\vec{x}_{m,a} \mid \vec{x}_{0,b}\right)_n \tag{73}$$

and

$$P_{ab}\left(m,t\right) \equiv \wp\left(\vec{x}_{m,a}, t \mid \vec{x}_{0,b}\right), \tag{74}$$

for $a, b = 1, 2, 3, \ldots, N_M$.

The derivation of basic random walk properties is facilitated by introducing the Fourier-Laplace transform $\tilde{\wp}^*\left(k, \vec{r}_a, s \mid \vec{x}_{0,b}\right)$ of the conditional probability $\wp\left(\vec{x}_{m,a}, t \mid \vec{x}_{0,b}\right)$. From equation (69), it can be easily shown that (see Appendix 1)

$$\tilde{\wp}^*\left(k, \vec{r}_a, s \mid \vec{x}_{0,b}\right) = \left(\frac{1 - \psi^*\left(s\right)}{s} \right) \tilde{\wp}\left(k, \vec{r}_a; \psi^*\left(s\right) \mid \vec{x}_{0,b}\right) \tag{75}$$

where $\tilde{\wp}\left(k,\vec{r}_a;\psi^*(s)\,|\,\vec{x}_{0,b}\right)$ is identical to the generating function $\tilde{\wp}\left(k,\vec{r}_a;\xi\,|\,\vec{x}_{0,b}\right)$ with ξ substituted by $\psi^*(s)$, and we have used the relations $\psi^*(s)_n=\left(\psi^*(s)\right)^n$ and $\Psi^*(s)=\dfrac{1-\psi^*(s)}{s}$.

In turn, from the concepts introduced in this thesis, i.e., the major sites and the associating multi-step transition probabilities $p\left(\vec{x}_{m,a},\vec{x}_{m-\Delta m,c}\right)_n$, the generating function $\tilde{\wp}\left(k,\vec{r}_a;\xi\,|\,\vec{x}_{0,b}\right)$, which plays a crucial role in our study, can be expressed in terms of these transition probabilities as follows.

Let us begin with the Chapman-Kolmogorov equation for the conditional probability of taking the n th step to a given site $\vec{x}_{m,a}$,

$$\wp\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_n=\delta_{n,0}\delta_{m,0}\delta_{a,b}+\sum_{n'=0}^{n}\sum_{c=1}^{N_M}\sum_{\Delta m=-1}^{1}p\left(\vec{x}_{m,a},\vec{x}_{m-\Delta m,c}\right)_{n'}P_{cb}\left(m-\Delta m\right)_{n-n'} \tag{76}$$

where $p\left(\vec{x}_{m,a},\vec{x}_{m-\Delta m,c}\right)_n$ is defined as the n-step transition probability from the major site $\vec{x}_{m-\Delta m,c}$ to the site $\vec{x}_{m,a}$, given that the walker does not visit any major site during the transition. The key idea of this equation is that the walker, which is found at the site $\vec{x}_{m,a}$ at the n th step, may be found at the major sites $\vec{x}_{m-\Delta m,c}$, for $c=1,2,3,...,N_M$ and $\Delta m=-1,0,1$, at any earlier $n-n'$ steps with the conditional probability $P_{cb}\left(m-\Delta m\right)_{n-n'}$. Then, for the remaining n' steps, it eventually walks to the given site $\vec{x}_{m,a}$ with the n'-step transition probabilities $p\left(\vec{x}_{m,a},\vec{x}_{m-\Delta m,c}\right)_{n'}$.

With the spatial homogeneity,

$$p\left(\vec{x}_{m,a},\vec{x}_{m-\Delta m,c}\right)_n=p\left(\vec{x}_{0,a},\vec{x}_{-\Delta m,c}\right)_n, \tag{77}$$

equation (76) can be rewritten as

$$\wp\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_n=\delta_{n,0}\delta_{m,0}\delta_{a,b}+\sum_{n'=0}^{n}\sum_{c=1}^{N_M}\sum_{\Delta m=-1}^{1}p\left(\vec{x}_{0,a},\vec{x}_{-\Delta m,c}\right)_{n'}P_{cb}\left(m-\Delta m\right)_{n-n'}. \tag{78}$$

The corresponding generating function of this equation is

$$\wp\left(\vec{x}_{m,a};\xi\,|\,\vec{x}_{0,b}\right)=\delta_{m,0}\delta_{a,b}+\sum_{c=1}^{N_M}\sum_{\Delta m=-1}^{1}p\left(\vec{r}_a,-\Delta mL\hat{x}+\vec{r}_c;\xi\right)P_{cb}\left(m-\Delta m;\xi\right) \tag{79}$$

where we have used the discrete convolution theorem. Then this equation is Fourier transformed. After rearranging (see Appendix 2), we obtain the resulting expression in the form

$$\tilde{\wp}\left(k,\vec{r}_a;\xi\,|\,\vec{x}_{0,b}\right)=\delta_{a,b}+\sum_{c=1}^{N_M}\overline{p}\left(k,\vec{r}_a,\vec{r}_c;\xi\right)\tilde{P}_{cb}\left(k;\xi\right) \tag{80}$$

where $\bar{p}(k,\vec{r}_a,\vec{r}_c;\xi)\equiv\sum_{\Delta m=-1}^{1}e^{ik\Delta mL}p(\vec{r}_a,-\Delta mL\hat{x}+\vec{r}_c;\xi)$. In turn, for $a,b=1,2,3,...,N_M$, the function $\tilde{P}_{ab}(k;\xi)$ satisfies the following relation:

$$\tilde{P}_{ab}(k;\xi)=\delta_{a,b}+\sum_{c=1}^{N_M}\bar{p}_{ac}(k;\xi)\tilde{P}_{cb}(k;\xi) \tag{81}$$

where $\bar{p}_{ac}(k;\xi)\equiv\sum_{\Delta m=-1}^{1}e^{ik\Delta mL}\left(\sum_{n=0}^{\infty}p_{ac}(\Delta m)_n\,\xi^n\right)$ and $p_{ac}(\Delta m)_n\equiv p(\vec{r}_a,-\Delta mL\hat{x}+\vec{r}_c)_n$ which is the n-step transition probability from a major site $\vec{x}_{-\Delta m,c}$ to the given major site $\vec{x}_{0,a}$, given that the walker does not visit any major site during the transition. This equation can be rewritten in a matrix form,

$$\tilde{\mathrm{P}}(k;\xi)=\mathrm{I}+\bar{\mathrm{p}}(k;\xi)\tilde{\mathrm{P}}(k;\xi) \tag{82}$$

where I is the $N_M\times N_M$ identity matrix,

$$\tilde{\mathrm{P}}(k;\xi)\equiv\begin{bmatrix}\tilde{P}_{11}(k;\xi) & \cdots & \tilde{P}_{1N_M}(k;\xi)\\ \vdots & \ddots & \vdots\\ \tilde{P}_{N_M1}(k;\xi) & \cdots & \tilde{P}_{N_MN_M}(k;\xi)\end{bmatrix}\text{ and }\bar{\mathrm{p}}(k;\xi)\equiv\begin{bmatrix}\bar{p}_{11}(k;\xi) & \cdots & \bar{p}_{1N_M}(k;\xi)\\ \vdots & \ddots & \vdots\\ \bar{p}_{N_M1}(k;\xi) & \cdots & \bar{p}_{N_MN_M}(k;\xi)\end{bmatrix}.$$

We have to note that, in this work, for any matrix A, we use $[\mathrm{A}]_{ab}$ or A_{ab}, A^{-1}, $\mathrm{adj}\,\mathrm{A}$, $\det\mathrm{A}$ and A^{T} as the notations for the entry in row a and column b, the inverse matrix, the adjugate matrix, the determinate and the transpose of A respectively.

Therefore, the solution of equation (82) can formally be written as

$$\tilde{\mathrm{P}}(k;\xi)=\left[\mathrm{I}-\bar{\mathrm{p}}(k;\xi)\right]^{-1} \tag{83}$$

or $\tilde{\mathrm{P}}(k;\xi)=\dfrac{\mathrm{adj}\left[\mathrm{I}-\bar{\mathrm{p}}(k;\xi)\right]}{\det\left[\mathrm{I}-\bar{\mathrm{p}}(k;\xi)\right]}$. Furthermore, it can be shown that $\det\left[\mathrm{I}-\bar{\mathrm{p}}(k;\xi)\right]$ and the eigenfunctions $E_n(k;\xi)$, for $n=1,2,3,...,N_M$, of the matrix $\bar{\mathrm{p}}(k;\xi)$ are related to each other by the relation (see Appendix 3)

$$\det\left[\mathrm{I}-\bar{\mathrm{p}}(k;\xi)\right]=\prod_{n=1}^{N_M}\left(1-E_n(k;\xi)\right). \tag{84}$$

Thus, the solution of equation (82) can also be calculated from

$$\tilde{\mathrm{P}}(k;\xi)=\frac{\mathrm{adj}\left[\mathrm{I}-\bar{\mathrm{p}}(k;\xi)\right]}{\prod_{n=1}^{N_M}\left(1-E_n(k;\xi)\right)}. \tag{85}$$

For consistency, if in each unity cell there exists only one major site, $N_M=1$, we will assign $\bar{\mathrm{p}}(k;\xi)=E_1(k;\xi)=\bar{p}_{11}(k;\xi)$ and $\mathrm{adj}\left[\mathrm{I}-\bar{\mathrm{p}}(k;\xi)\right]=1$.

Consequently, from the previous description, we can express an exact analytical expression for the Fourier-Laplace transform $\tilde{\wp}^*\left(k,\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)$ in terms of the mesoscopic characteristics of random walks on the quasi-1d lattices, namely the transition probabilities $p\left(\vec{r}_a,-\Delta mL\hat{x}+\vec{r}_c\right)_n$ and the PDF of waiting time $\psi(t)$, i.e.,

$$\tilde{\wp}^*\left(k,\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)=\left(\frac{1-\psi^*(s)}{s}\right)\tilde{\wp}\left(k,\vec{r}_a;\psi^*(s)\,|\,\vec{x}_{0,b}\right) \tag{86}$$

where

$$\tilde{\wp}\left(k,\vec{r}_a;\xi\,|\,\vec{x}_{0,b}\right)=\delta_{a,b}+\sum_{c=1}^{N_M}\bar{p}\left(k,\vec{r}_a,\vec{r}_c;\xi\right)\frac{\mathrm{adj}\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(k;\xi\right)\right]_{cb}}{\prod_{n=1}^{N_M}\left(1-E_n\left(k;\xi\right)\right)}. \tag{87}$$

In addition to the Fourier-Laplace transform $\tilde{\wp}^*\left(k,\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)$, the Laplace transforms of the conditional probability $\wp\left(\vec{x}_{m,a},t\,|\,\vec{x}_{0,b}\right)$ and of the conditional first-passage probability (CFPP) $\mathcal{F}\left(\vec{x}_{m,a},t\,|\,\vec{x}_{0,b}\right)$ to a given site $\vec{x}_{m,a}$ at time t are also used to derive a number of basic statistical properties of the random walk. The CFPP $\mathcal{F}\left(\vec{x}_{m,a},t\,|\,\vec{x}_{0,b}\right)$ is given by

$$\mathcal{F}\left(\vec{x}_{m,a},t\,|\,\vec{x}_{0,b}\right)=\sum_{n=0}^{\infty}\mathcal{F}\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_n\psi(t)_n \tag{88}$$

where $\mathcal{F}\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_n$ is the CFPP to the site $\vec{x}_{m,a}$ at the nth step. On the other hand, the Laplace transform $\wp^*\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right)$ can be calculated by performing inverse Fourier transformation of $\tilde{\wp}^*\left(k,\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)$,

$$\wp^*\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right)=\left(\frac{1-\psi^*(s)}{s}\right)\frac{L}{2\pi}\int_{-\pi/L}^{\pi/L}e^{-ikmL}\tilde{\wp}\left(k,\vec{r}_a;\psi^*(s)\,|\,\vec{x}_{0,b}\right)dk. \tag{89}$$

From equation (88), it can be shown without any difficulties that the Laplace transform $\mathcal{F}^*\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right)$ is identical to the generating function $\mathcal{F}\left(\vec{x}_{m,a};\psi^*(s)\,|\,\vec{x}_{0,b}\right)$ with ξ substituted by $\psi^*(s)$, i.e.,

$$\mathcal{F}^*\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right)=\mathcal{F}\left(\vec{x}_{m,a};\psi^*(s)\,|\,\vec{x}_{0,b}\right) \tag{90}$$

where the relation $\psi^*(s)_n=\left(\psi^*(s)\right)^n$ was used. In addition, it can be demonstrated that the generating function $\mathcal{F}\left(\vec{x}_{m,a};\xi\,|\,\vec{x}_{0,b}\right)$ has a simple relation to the generating function $\wp\left(\vec{x}_{m,a};\xi\,|\,\vec{x}_{0,b}\right)$. First consider another expression of $\wp\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_n$,

$$\wp\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_n=\delta_{m,0}\delta_{a,b}\delta_{n,0}+\sum_{n'=0}^{n}\wp\left(\vec{x}_{m,a}\,|\,\vec{x}_{m,a}\right)_{n'}\mathcal{F}\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_{n-n'}. \tag{91}$$

The idea is: the conditional probability of a walker being found at a site $\vec{x}_{m,a}$ after n steps equals to the sum of all probabilities that the walker is found at that site for the first time at any earlier $n-n'$ steps and, the rest of its walk, it can go anywhere on the structure but eventually it must be found at that site. Then find the corresponding generating function. After rearrangement, we obtain

$$\mathcal{F}\left(\vec{x}_{m,a};\xi \mid \vec{x}_{0,b}\right)=\frac{\wp\left(\vec{x}_{m,a};\xi \mid \vec{x}_{0,b}\right)-\delta_{m,0}\delta_{a,b}}{\wp\left(\vec{x}_{0,a};\xi \mid \vec{x}_{0,a}\right)} \tag{92}$$

where the relation $\wp\left(\vec{x}_{0,a};\xi \mid \vec{x}_{0,a}\right)=\wp\left(\vec{x}_{m,a};\xi \mid \vec{x}_{m,a}\right)$ was exploited.

In general, the Laplace transform $\wp^*\left(\vec{x}_{m,a},s \mid \vec{x}_{0,b}\right)$ for an arbitrary site $\vec{x}_{m,a}$ in equation (89) is somewhat complicated for further analysis. On the other hand, if the considered site is a major site $\vec{x}_{m,a}$, for $a=1,2,3,...,N_M$, the Laplace transform is easier for further analysis and it can be calculated from

$$P^*_{ab}\left(m,s\right)=\left(\frac{1-\psi^*\left(s\right)}{s}\right)P_{ab}\left(m;\psi^*\left(s\right)\right), \tag{93}$$

$$P_{ab}\left(m;\xi\right)=\frac{L}{2\pi}\int_{-\pi/L}^{\pi/L}e^{-ikmL}\frac{\mathrm{adj}\left[\mathrm{I}-\bar{\mathrm{p}}\left(k;\xi\right)\right]_{ab}}{\prod_{n=1}^{N_M}\left(1-E_n\left(k;\xi\right)\right)}dk\,. \tag{94}$$

As we have learned from equations (90) and (92), if this integral can be calculated, then the Laplace transform $F^*_{ab}\left(m,s\right)\equiv\mathcal{F}^*\left(\vec{x}_{m,a},s \mid \vec{x}_{0,b}\right)$ of the associating CFPP $F_{ab}\left(m,t\right)\equiv\mathcal{F}\left(\vec{x}_{m,a},t \mid \vec{x}_{0,b}\right)$, for $a=1,2,3,...,N_M$, is immediate,

$$F^*_{ab}\left(m,s\right)=\frac{P_{ab}\left(m;\psi^*\left(s\right)\right)-\delta_{m,0}\delta_{a,b}}{P_{aa}\left(0;\psi^*\left(s\right)\right)}\,. \tag{95}$$

To sum up, we have derived the expressions of the Fourier-Laplace transform $\tilde{\wp}^*\left(k,\vec{r}_a,s \mid \vec{x}_{0,b}\right)$ and the Laplace transforms $P^*_{ab}\left(m,s\right)$ and $F^*_{ab}\left(m,s\right)$ in terms of the mesoscopic characteristics of the random walk on the quasi-1d lattices, namely the multi-step transition probabilities $p\left(\vec{x}_{0,a},\vec{x}_{\Delta m,b}\right)_n$ and the PDF of waiting time $\psi\left(t\right)$.

In the next section, we will show that equations (86) and (87) together with the fundamental generating functions, i.e., $p_{ab}\left(\Delta m;\xi\right)$ for $a,b=1,2,3,...,N_M$ and $\Delta m=-1,0,1$, can be used to find the asymptotic behavior of the first two moments of the walker location along the structure axis. Analogously, equations (93) - (95) and the fundamental generating functions allow us to obtain various other random walk properties for a given major site.

2.3 Asymptotic behavior of basic random walk properties

We introduce here basic statistical properties of the SCTRW on quasi-1d infinite structures and present a systematic approach to calculate them by exploiting the general formalism developed in the previous section. Since the approach is based on the concept of generating functions, which makes working with the asymptotic behavior of random walk properties very convenient, we will call it the generating function formalism (GFF) from now on.

The random walk properties considered in this thesis include the first and the second moments of a walker location along the structure axis at certain times, the probability of return to the starting site at certain times, the probability of ever reaching a given major site, the conditional mean first-passage times to a given major site and the expected number of distinct major sites visited at certain times. As you have seen in the introduction, these statistical random walk properties are commonly considered because they play a central role in the basic description of the random motion of a walker on lattice structures.

In general, there are few random walks for which the exact closed-form evaluation of these basic statistical properties can be found. Even when it is possible to calculate them exactly, their formulae may be somewhat complicated. Thus, useful information is extractable from them only by introducing some forms of approximations. Therefore, we will hereafter focus on the long-time behavior of the basic statistical properties. To analyze this behavior, the asymptotic behavior of the Laplace transform $\psi^*(s)$ of the PDF $\psi(t)$ of waiting time as $s \to 0^+$ is of concerned.

Before proceeding to discuss the basic random walk properties, we pause to discuss the PDF $\psi(t)$ of waiting time in more detail. If steps of a walker are taken at certain times $t_0, 2t_0, 3t_0, \ldots$ instead of random times, the PDF of waiting time is in the form of the delta function,

$$\psi(t) = \delta(t - t_0), \tag{96}$$

and its Laplace transform is

$$\psi^*(s) = e^{-st_0}. \tag{97}$$

The corresponding random walks are known as the discrete-time random walks with the waiting time $t_0 > 0$. The canonical case of the continuous time random walk is the exponential waiting-time density,

$$\psi(t) = \lambda \exp(-\lambda t) \tag{98}$$

whose Laplace transform is

$$\psi^*(s) = \frac{\lambda}{\lambda + s}. \tag{99}$$

It is not hard to show that the mean waiting time is equal to λ^{-1}.

Working with a more general PDF of waiting time allows us to derive a number of informative results which are concealed in an analysis restricted to the exponential distribution function. In what follows, we paraphrase some arguments from the work of Bendler and Shlesinger [42] with the corresponding adaptation to the analysis of a more general PDF of waiting time.

Consider the walker waiting time at a site on the underlying structure from a potential point of view, where the intrinsic properties of the site can be related to a potential U in some way. We assume that the PDF of waiting time arises from a superposition of exponential PDF,

$$\psi(t) = \int_0^{\lambda_0} \rho(\lambda) \lambda \exp(-\lambda t) d\lambda \tag{100}$$

where $\rho(\lambda) = f(U(\lambda)) \left| dU(\lambda)/d\lambda \right|$. The rate constant λ satisfies the classical formula for thermally activated crossing of an energy barrier of height $U \geq 0$,

$$\lambda = \lambda_0 \exp(-U/kT) \tag{101}$$

where T is the absolute temperature, k is Boltzmann's constant and λ_0 is the highest value of the rate constant associated with the minimum energy barrier height $U = 0$. The further assumption is that the potential U is random and distributed by the exponential law

$$f(U) = \frac{1}{\langle U \rangle} \exp\left(-\frac{U}{\langle U \rangle} \right) \tag{102}$$

where $\langle U \rangle$ is the mean of the energy barrier height. Therefore, from equation (100) – (102), we can find

$$\rho(\lambda) = \frac{\nu}{\lambda} \left(\frac{\lambda}{\lambda_0} \right)^{\nu} \tag{103}$$

where $0<\lambda\le\lambda_0$ and $v\equiv kT/\langle U\rangle$. In the limits that $0<v<1$ and λ_0 is large, the asymptotic forms of the PDF $\psi(t)$ and its Laplace transform $\psi^*(s)$ become

$$\psi(t)\sim\frac{v\Gamma(1+v)}{\lambda_0^v}t^{-1-v}, \tag{104}$$

$$\psi^*(s)\sim 1-(t_0 s)^v \tag{105}$$

where $t_0^v=\frac{v\pi}{\lambda_0^v\sin(v\pi)}$. This kind of PDFs is known as the heavy-tailed PDF. One crucial fact about this PDF is that all of its moments are infinite.

In this work, for analysis completeness, we will take into account general PDFs of waiting time whose Laplace transforms are in the asymptotic form

$$\psi^*(s)\sim 1-(t_0 s)^v \tag{106}$$

where s is small and $0<v\le 1$. The equality is for the finite mean PDFs. In this case, t_0 is equal to the mean waiting time, i.e., $t_0=\int_0^\infty t\psi(t)\,dt$. The inequality is for the infinite mean PDFs and $t_0^v=\frac{v\pi}{\lambda_0^v\sin(v\pi)}$. In numerical simulations, for the former and the latter cases, we use the exponential and the heavy-tailed PDFs, which obey equations (98) and (104), respectively.

Incidentally, for a function $f(\psi^*(s))$ with the argument ξ substituted by the Laplace transform $\psi^*(s)$, the investigation of the limit of this function as $s\to 0^+$ is equivalent to the investigation of the limit of the function $f(\xi)$ as $\xi\to 1^-$ because $\psi^*(s)\to 1^-$ as $s\to 0^+$. In addition, to avoid a lot of unnecessary writing, we will use the shorthand notations for (i) the limit of the function as $\xi\to 1^-$, say $\lim_{\xi\to 1^-}f(\xi)$, by omitting its argument, i.e., f, or replacing its argument by 1^-, i.e., $f(1^-)$, and (ii) the derivative $\frac{\partial f(\xi)}{\partial\xi}$ by $(f(\xi))'$.

As we shall see later, the asymptotic behavior of the basic statistical properties is also governed by the behavior of the eigenfunctions and the eigenvectors of the matrix $\overline{\mathrm{p}}(k;\xi)$ near the point $(k,\xi)=(0,1)$. From the definition, the matrix $\overline{\mathrm{p}}(0;1^-)$ can be interpreted as the transition probability matrix of the embedded Markov chain which is resulted from the projection of the random walk on the set of non-equivalent major sites of the corresponding model. Thus, the

embedded Markov chain is a stochastic process that takes on N_M number of possible states (major sites), and whenever the process is in state b, there is a transition probability $\bar{p}_{ab}\left(0;1^-\right)$ that it will next be in state a, for $a,b=1,2,3,...,N_M$.

In this work, we mainly consider the random walk models with the matrix $\bar{\mathrm{p}}\left(k;\xi\right)$ whose limit $\bar{\mathrm{p}}\left(0;1^-\right)$ is the transition matrix of an irreducible and aperiodic Markov chain [54]. To clarify this statement, let us consider the relation $\bar{\mathrm{p}}\left(k;\xi\right)\pi\left(k;\xi\right)=E_1\left(k;\xi\right)\pi\left(k;\xi\right)$ which gives

$$E_1\left(k;\xi\right)=\frac{\sum_{a,b=1}^{N_M}\bar{p}_{ab}\left(k;\xi\right)\pi_b\left(k;\xi\right)}{\sum_{b=1}^{N_M}\pi_b\left(k;\xi\right)} \tag{107}$$

where $E_1\left(k;\xi\right)$ and $\pi\left(k;\xi\right)\equiv\left[\pi_1\left(k;\xi\right)\ \ \ldots\ \ \pi_{N_M}\left(k;\xi\right)\right]^{\mathrm{T}}$ are the eigenfunction and the eigenvector of the matrix $\bar{\mathrm{p}}\left(k;\xi\right)$. The irreducibility and the aperiodicity imply that the limits $E_1\left(0;1^-\right)$ and $\sum_{a=1}^{N_M}\pi_a\left(0;1^-\right)$ equal to unity. The physical meaning of the entry $\pi_a\equiv\pi_a\left(0;1^-\right)$ is the limiting probability that a walker is at a major site a at large steps. Hence, from equation (107), we shall claim that, at the point that $k=0$, the eigenfunction $E_1\left(0;\xi\right)$ is nothing but the generating function of the probability that, after commencing from a certain major site, the walker is found at near major sites or the commencing site itself after certain steps for first time.

For the rest of this thesis, the random walk model with $E_1\left(0;1^-\right)=1$ will be called the diffusive random walk (DRW). This means that the random walker repeatedly visits major sites, and it is able to diffuse along the structure axis. In other words, it will not get lost and stuck in a connected network. In contrast, if it can get lost and stuck in a connected network, i.e., $0<E_1\left(0;1^-\right)<1$, the model will be called the non-diffusive random walk (NDRW).

Since, after sufficiently long time, NDRW gets lost in some connected network and the averages of the dynamical properties along the structure axis are frozen at certain constants, we restrict ourselves in this work to DRWs whose dynamical properties evolve in time.

Additionally, if $\bar{\mathrm{p}}\left(0;1^{-}\right)$ is the transition matrix of an irreducible and aperiodic Markov chain, then we can show that the entries of the limit eigenvector $\pi \equiv \pi\left(0;1^{-}\right)$ are identical to the following equation (see Appendix 4)

$$\pi_a = \frac{\left[\mathrm{adj}\left(\mathrm{I}-\bar{\mathrm{p}}\left(0;1^{-}\right)\right)\right]_{ab}}{\prod_{n=2}^{N_M}\left(1-E_n\left(0;1^{-}\right)\right)} \tag{108}$$

for $a,b=1,2,3,\ldots,N_M$.

2.3.1 The first and the second moments

To characterize a transport of a random walk on certain kind of structures, we need a quantity statistically indicating the walker location on the structure, e.g., the moments of the walker location on the structure after certain times. In our models, the first and the second moments of the random walker location along the structure axis are of our interest.

The first moment $\langle x\rangle(t)$ and the second moment $\langle x^2\rangle(t)$ of the random walker location along the structure axis at time t, given that the random walker initiated at a starting site $\vec{x}_{0,b}$, are defined by

$$\langle x\rangle(t) \equiv \sum_{m=-\infty}^{\infty}\sum_{a=1}^{N} x_{m,a}\wp\left(\vec{x}_{m,a},t\,|\,\vec{x}_{0,b}\right) \tag{109}$$

and

$$\langle x^2\rangle(t) \equiv \sum_{m=-\infty}^{\infty}\sum_{a=1}^{N} x_{m,a}^2\wp\left(\vec{x}_{m,a},t\,|\,\vec{x}_{0,b}\right). \tag{110}$$

To determine the asymptotic behavior of these two moments at large time t, let us consider their Laplace transforms $\langle x\rangle^{*}(s)$ and $\langle x^2\rangle^{*}(s)$. The Laplace transforms of these moments can be calculated from (see Appendix 5)

$$\langle x\rangle^{*}(s) = \frac{1}{i}\frac{\partial}{\partial k}\sum_{a=1}^{N} e^{ik\hat{x}\bullet\vec{r}_a}\tilde{\wp}^{*}\left(k,\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)\Big|_{k=0} \tag{111}$$

and

$$\langle x^2\rangle^{*}(s) = \frac{1}{i^2}\frac{\partial^2}{\partial k^2}\sum_{a=1}^{N} e^{ik\hat{x}\bullet\vec{r}_a}\tilde{\wp}^{*}\left(k,\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)\Big|_{k=0}. \tag{112}$$

For the first moment, substitution of equation (86) into equation (111) yields

$$\begin{aligned}\langle x\rangle^{*}(s) &= \left(\frac{1-\psi^{*}(s)}{s}\right)\left\{\hat{x}\bullet\vec{r}_b+\sum_{a=1}^{N}\sum_{c=1}^{N_M}\frac{\partial}{i\partial k}e^{ik\hat{x}\bullet\vec{r}_a}\,\overline{p}\left(k,\vec{r}_a,\vec{r}_c;\psi^{*}(s)\right)\Big|_{k=0}\tilde{P}_{cb}\left(0;\psi^{*}(s)\right)\right.\\ &\left.+\sum_{a=1}^{N}\sum_{c=1}^{N_M}\overline{p}\left(0,\vec{r}_a,\vec{r}_c;\psi^{*}(s)\right)\frac{\partial}{i\partial k}\tilde{P}_{cb}\left(k;\psi^{*}(s)\right)\Big|_{k=0}\right\}\end{aligned} \tag{113}$$

where the generating function $\tilde{P}_{cb}\left(k;\psi^{*}(s)\right)$ is determined by equation (85). For DRWs, the term $\left(1-E_1\left(k;\psi^{*}(s)\right)\right)^{-1}$ in the generating function $\tilde{P}_{cb}\left(k;\psi^{*}(s)\right)$ is divergent as $(k,s)\to(0,0)$ so the third term in equation (113) is the dominant term and only important if no change happens,

$$\langle x\rangle^{*}(s)\sim\left(\frac{1-\psi^{*}(s)}{s}\right)\sum_{a=1}^{N}\sum_{c=1}^{N_M}\overline{p}\left(0,\vec{r}_a,\vec{r}_c;\psi^{*}(s)\right)\frac{\partial}{i\partial k}\tilde{P}_{cb}\left(k;\psi^{*}(s)\right)\Big|_{k=0} \tag{114}$$

where the asymptotic form of the derivative can be found in the following expression:

$$\frac{\partial}{i\partial k}\tilde{P}_{ab}\left(k;\psi^{*}(s)\right)\Big|_{k=0}\sim\frac{\mathrm{adj}\left[\mathrm{I}-\overline{\mathrm{p}}\left(0;\psi^{*}(s)\right)\right]_{ab}}{\prod_{n=2}^{N_M}\left(1-E_n\left(0;\psi^{*}(s)\right)\right)}\frac{\frac{\partial}{i\partial k}E_1\left(k;\psi^{*}(s)\right)\Big|_{k=0}}{\left(1-E_1\left(0;\psi^{*}(s)\right)\right)^{2}}. \tag{115}$$

If we plug equation (115) into equation (114), we will get the complicated equation. To make it less complicated, let us consider the sum $\sum_{a=1}^{N}\tilde{\wp}^{*}\left(0,\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)$. From the definition, it is expressed as

$$\sum_{a=1}^{N}\tilde{\wp}^{*}\left(0,\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)=\int_0^{\infty}\left(\sum_{m=-\infty}^{\infty}\sum_{a=1}^{N}\wp\left(\vec{x}_{m,a},t\,|\,\vec{x}_{0,b}\right)\right)e^{-st}dt. \tag{116}$$

From the fact that the random walker cannot be eliminated from the system or the walker must be found somewhere on the structure at any given time, we have $\sum_{m=-\infty}^{\infty}\sum_{a=1}^{N}\wp\left(\vec{x}_{m,a},t\,|\,\vec{x}_{0,b}\right)=1$ for any time t. Hence, $\sum_{a=1}^{N}\tilde{\wp}^{*}\left(0,\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)=\frac{1}{s}$ for $s>0$. This result, equations (86) and (87) lead to the relation (see Appendix 6)

$$\frac{1-E_1\left(0;\psi^{*}(s)\right)}{1-\psi^{*}(s)}\sim\sum_{a=1}^{N}\sum_{c=1}^{N_M}\overline{p}\left(0,\vec{r}_a,\vec{r}_c;\psi^{*}(s)\right)\frac{\mathrm{adj}\left[\mathrm{I}-\overline{\mathrm{p}}\left(0;\psi^{*}(s)\right)\right]_{cb}}{\prod_{n=2}^{N_M}\left(1-E_n\left(0;\psi^{*}(s)\right)\right)}. \tag{117}$$

After substituting equation (115) into equation (114) and using relation (117), we find

$$\langle x\rangle^{*}(s)\sim\frac{1}{s\left(1-E_1\left(0;\psi^{*}(s)\right)\right)}\frac{\partial}{i\partial k}E_1\left(k;\psi^{*}(s)\right)\Big|_{k=0}. \tag{118}$$

We will restrict ourselves to the DRWs with the asymptotic form of the eigenfunction $E_1(0;\xi)$ as $\xi \to 1^-$ obeying the equation

$$1-E_1(0;\xi) \sim c_1(1-\xi)^{2-d_H} \tag{119}$$

where c_1 is a certain constant and $1 \le d_H < 2$. We defer further discussion of the meaning of the parameter d_H until the next subsection.

We can show that if the expected number G of steps that the random walker takes inside connected networks before returning to any major site again is finite, then the asymptotic form of the term $1-E_1(0;\xi)$ satisfies the above equation,

$$1-E_1(0;\xi) \sim G(1-\xi) \tag{120}$$

where $c_1 = G$ and $d_H = 1$ (see appendix 7). The expected number G can be calculated from the limit as $\xi \to 1^-$ of the derivative of the eigenfunction $E_1(0;\xi)$ with respect to ξ,

$$G = \left(E_1\left(0;1^-\right)\right)' \tag{121}$$

which is also equal to $\sum_{b=1}^{N_M}\left(1+\sum_{a=1}^{N_M}\bar{p}_{ab}\left(0;1^-\right)\right)\pi_b$. The corresponding random walk is denominated the diffusive random walk with finite G (DRWFG). On the other hand, if the dangling networks attached to major sites are fractals with dimension in the interval $(0,2)$ and the walker takes symmetrically steps on such networks, then the expected number G is infinite and the parameter $d_H > 1$. The corresponding random walk is called the DRW with infinite G (DRWFIG).

For DRWs, from equations (106) and (119), the asymptotic form of the Laplace transform $\langle x\rangle^*(s)$ in equation (118) therefore becomes

$$\langle x\rangle^*(s) \sim \frac{\Gamma\left(1+\nu\left(2-d_H\right)\right)\vartheta}{s^{1+\nu(2-d_H)}} \tag{122}$$

where $\vartheta \equiv \frac{1}{\Gamma\left(1+\nu\left(2-d_H\right)\right)c_1 t_0^{\nu(2-d_H)}}\left(\frac{\partial}{i\partial k}E_1\left(k;1^-\right)\Big|_{k=0}\right)$ is called the effective velocity. The gamma function $\Gamma\left(1+\nu\left(2-d_H\right)\right)$ is introduced in order to simplify some of the further expressions. From equation (107), it can be shown that the effective velocity can also be calculated from

$$\vartheta = \frac{1}{\Gamma\left(1+\nu\left(2-d_H\right)\right)c_1 t_0^{\nu(2-d_H)}}\sum_{a,b=1}^{N_M}\left(\frac{\partial}{i\partial k}\bar{p}_{ab}\left(k;1^-\right)\Big|_{k=0}\right)\pi_b . \tag{123}$$

Note that when the term “unbiased random walk” (“biased random walk”) is used here, it will be understood that we refer specifically that $\mathcal{G}=0$ ($\mathcal{G}\neq 0$) unless we say otherwise.

After obtaining the asymptotic form of the Laplace transform in equation (122), we can find the asymptotic form of the first moment $\langle x\rangle(t)$ by applying Tauberian theorem to it,

$$\langle x\rangle(t)\sim \mathcal{G}t^{\nu(2-d_H)}. \tag{124}$$

Tauberian theorem states that, for a function $f(t)$ and its Laplace transform $f^*(s)\equiv\int_0^\infty f(t)e^{-st}dt$,

$$f^*(s)\sim s^{-\rho}L\left(\frac{1}{s}\right) \text{ as } s\to 0^+, \text{ and } f(t)\sim\frac{t^{\rho-1}}{\Gamma(\rho)}L(t) \text{ as } t\to\infty$$

are equivalent, provided that $\rho>0$, $\Gamma(\rho)$ is gamma function, $f(t)$ is always positive and monotonic, and the function $L(x)$ is slowly varying in the sense that $\frac{L(\lambda x)}{L(x)}\to 1$ as $x\to\infty$ for each fixed, positive λ.

The analysis of the asymptotic behavior of the second moment $\langle x^2\rangle(t)$ is analogous to one of the first moment $\langle x\rangle(t)$. First determine the Laplace transform $\langle x^2\rangle^*(s)$ by substituting equation (86) into equation (112),

$$\begin{aligned}\langle x^2\rangle^*(s)=&\left(\frac{1-\psi^*(s)}{s}\right)\Big\{\left(\hat{x}\bullet\vec{r}_b\right)^2\\&+\sum_{a=1}^{N}\sum_{c=1}^{N_M}\frac{\partial^2}{i^2\partial k^2}e^{ik\hat{x}\bullet\vec{r}_a}\,\bar{p}\left(k,\vec{r}_a,\vec{r}_c;\psi^*(s)\right)\Big|_{k=0}\tilde{P}_{cb}\left(0;\psi^*(s)\right)\\&+\frac{2}{i^2}\sum_{a=1}^{N}\sum_{c=1}^{N_M}\frac{\partial}{\partial k}e^{ik\hat{x}\bullet\vec{r}_a}\,\bar{p}\left(k,\vec{r}_a,\vec{r}_c;\psi^*(s)\right)\Big|_{k=0}\frac{\partial}{\partial k}\tilde{P}_{cb}\left(k;\psi^*(s)\right)\Big|_{k=0}\\&+\sum_{a=1}^{N}\sum_{c=1}^{N_M}\bar{p}\left(0,\vec{r}_a,\vec{r}_c;\psi^*(s)\right)\frac{\partial^2}{i^2\partial k^2}\tilde{P}_{cb}\left(k;\psi^*(s)\right)\Big|_{k=0}\Big\}\end{aligned}. \tag{125}$$

For DRWs, the last term of this equation is the leading term as $s\to 0^+$,

$$\langle x^2\rangle^*(s)\sim\left(\frac{1-\psi^*(s)}{s}\right)\sum_{a=1}^{N}\sum_{c=1}^{N_M}\bar{p}\left(0,\vec{r}_a,\vec{r}_c;\psi^*(s)\right)\frac{\partial^2}{i^2\partial k^2}\tilde{P}_{cb}\left(k;\psi^*(s)\right)\Big|_{k=0}. \tag{126}$$

From equation (85), the dominant contribution to the second derivative in equation (126) reads

$$\left.\frac{\partial^2}{i^2\partial k^2}\tilde{P}_{cb}\left(k;\psi^*(s)\right)\right|_{k=0} \sim \frac{\mathrm{adj}\left[\mathrm{I}-\bar{\mathrm{p}}\left(0;\psi^*(s)\right)\right]_{ab}}{\prod_{n=2}^{N_M}\left(1-E_n\left(0;\psi^*(s)\right)\right)}\left\{\frac{2\left(\left.\frac{\partial}{i\partial k}E_1\left(k;\psi^*(s)\right)\right|_{k=0}\right)^2}{\left(1-E_1\left(0;\psi^*(s)\right)\right)^3}\right.$$
$$\left.+\frac{\left.\frac{\partial^2}{i^2\partial k^2}E_1\left(k;\psi^*(s)\right)\right|_{k=0}}{\left(1-E_1\left(0;\psi^*(s)\right)\right)^2}\right\}. \quad (127)$$

If equations (117) and (127) are used, it is easily shown that equation (126) becomes

$$\left\langle x^2\right\rangle^*(s) \sim \frac{1}{s}\left\{\frac{2\left(\left.\frac{\partial}{i\partial k}E_1\left(k;\psi^*(s)\right)\right|_{k=0}\right)^2}{\left(1-E_1\left(0;\psi^*(s)\right)\right)^2}+\frac{\left.\frac{\partial^2}{i^2\partial k^2}E_1\left(k;\psi^*(s)\right)\right|_{k=0}}{\left(1-E_1\left(0;\psi^*(s)\right)\right)}\right\}. \quad (128)$$

After plugging equations (106) and (119) into equation (128), we find that the asymptotic form of the Laplace transform $\left\langle x^2\right\rangle^*(s)$ is

$$\left\langle x^2\right\rangle^*(s) \sim \frac{2\left(\Gamma\left(1+\nu\left(2-d_H\right)\right)\vartheta\right)^2}{s^{2\nu(2-d_H)+1}}+\frac{2\Gamma\left(1+\nu\left(2-d_H\right)\right)D}{s^{1+\nu(2-d_H)}} \quad (129)$$

where $D \equiv \frac{1}{2\Gamma\left(1+\nu\left(2-d_H\right)\right)c_1 t_0^{\nu(2-d_H)}}\left(\left.\frac{1}{i^2}\frac{\partial^2}{\partial k^2}E_1\left(k;1^-\right)\right|_{k=0}\right)$ is called the diffusion coefficient. From equation (107), we can find that, in the case of unbiased random walks, the diffusion coefficient can also be calculated from

$$D=\frac{1}{2\Gamma\left(1+\nu\left(2-d_H\right)\right)c_1 t_0^{\nu(2-d_H)}}\sum_{a,b=1}^{N_M}\left(\left.\frac{\partial^2}{i^2\partial k^2}\bar{p}_{ab}\left(k;1^-\right)\right|_{k=0}\right)\pi_b . \quad (130)$$

Finally, after applying Tauberian theorem to equation (129), the asymptotic form of the second moment $\left\langle x^2\right\rangle(t)$ is obtained,

$$\left\langle x^2\right\rangle(t) \sim \frac{2\Gamma^2\left(1+\nu\left(2-d_H\right)\right)}{\Gamma\left(1+2\nu\left(2-d_H\right)\right)}\left\langle x\right\rangle^2(t)+2Dt^{\nu(2-d_H)} . \quad (131)$$

In summary, from the preceding analysis, we have found that, for DRWs, if the explicit forms of the eigenfunction $E_1\left(k;\xi\right)$ and the eigenvector $\pi\left(k;\xi\right)$ of the transition probability matrix $\bar{\mathrm{p}}\left(k;\xi\right)$ are known, then the asymptotic forms of the Laplace transforms $\left\langle x\right\rangle^*(s)$ and $\left\langle x^2\right\rangle^*(s)$ as $s\to 0^+$ can be calculated. Furthermore, if these asymptotic forms satisfy the conditions of Tauberian theorem, then we will

easily find the asymptotic forms of the first moment $\langle x \rangle(t)$ and the second moment $\langle x^2 \rangle(t)$ of the random walker location along the structure axis at large time t.

For the DRWFGs, $G < \infty$ and $d_H = 1$, we found that the asymptotic behavior of these moment is identical to those for the random walk on a perfect 1-d lattice except for the coefficients – the effective velocity ϑ and the diffusion coefficient D. For the unbiased DRWFGs, the second moment $\langle x^2 \rangle(t)$ is proportional to time t if the PDF of waiting time has a finite mean, i.e., $\nu = 1$. Otherwise, the second moment is proportional to t^{ν} for $0 < \nu < 1$ instead. In words, the only diffusion of the unbiased DRWFGs with the PDF of waiting time possessing the finite mean is a normal diffusion. If this condition, i.e., $\nu = 1$, is relaxed, it leads to the field of anomalous diffusions. Realistic models of anomalous diffusion have been formulated for nonlinear transport in disordered materials (see, e.g., [10]).

Just before we move on, it is important to remark that the asymptotic behavior of the other basic properties can also be obtained by applying the Tauberian theorem to their corresponding Laplace transforms, so we often implicitly use this fact.

2.3.2 The probability of return to the starting site

The basic problem of the theory of random walks is to calculate the probability of a walker being found at a certain time and a certain site, e.g., the starting site. For the models with the spatial homogeneity, aside from the other basic statistical properties of a random walk for a given site, the probability $P_{bb}(0)_n$ that the walker is found at the starting site at the nth is related to many interesting problems such as the lattice vibration problem on the same lattice structure [55] , the relaxation process described by the defect-diffusion model [56] and recurrence theorem [57]. For the continuous-time random walks, the conditional probability $P_{bb}(0)_n$ can be generalized to the probability $P_{bb}(0,t)$ of return to the starting site $\vec{x}_{0,b}$ at time t.

Since the probability $P_{bb}(0,t)$ is the special case of the probability $P_{ab}(m,t)$ that the walker is found at any major site $\vec{x}_{m,a}$ at time t, let us begin our consideration with equations (93) and (94) for $m = 0$ and $a = b$, i.e.,

$$P_{bb}^{*}(0,s)=\left(\frac{1-\psi^{*}(s)}{s}\right)P_{bb}\left(0;\psi^{*}(s)\right) \tag{132}$$

and $P_{bb}(0;\xi)=\dfrac{L}{2\pi}\displaystyle\int_{-\pi/L}^{\pi/L}\frac{\mathrm{adj}\left[\mathrm{I}-\bar{\mathrm{p}}(k;\xi)\right]_{bb}}{\displaystyle\prod_{n=1}^{N_M}\left(1-E_n(k;\xi)\right)}dk$ which can also be calculated from

$$P_{bb}(0;\xi)=\frac{1}{2\pi i}\oint_{\mathcal{C}}\frac{\mathrm{adj}\left[\mathrm{I}-\bar{\mathrm{p}}(k(z);\xi)\right]_{bb}}{\displaystyle\prod_{n=1}^{N_M}\left(1-E_n(k(z);\xi)\right)}\frac{dz}{z} \tag{133}$$

where $z\equiv e^{iLk}$ and the contour $\mathcal{C}$ is the unit circle.

The singularities $z_{-}^{(i)}(\xi)$ of the integrand are located at the points in a complex z plane where $1-E_n\left(k\left(z_{-}^{(i)}(\xi)\right);\xi\right)=0$ for $n=1,2,3,...,N_M$. For a great number of problems, it can be shown that these singularities are poles. Hence, let us restrict ourselves to this kind of the problems.

As admitted above, there may exist a certain number I of poles in the region bounded by the contour $\mathcal{C}$, and the residue theorem yields

$$P_{bb}(0;\xi)=\sum_{i=1}^{I}P_{bb}^{(i)}(\xi)_{-} \tag{134}$$

where the term $P_{bb}^{(i)}(\xi)_{-}$ corresponds to the pole $z_{-}^{(i)}(\xi)$ for $i=1,2,3,...,I$. The meaning of the minus sign subscript will be clarified later.

For DRWs, for ease of reference, let us preserve the notation $z_{-}^{(1)}(\xi)$ for the pole corresponding to $1-E_1\left(k\left(z_{-}^{(1)}(\xi)\right);\xi\right)=0$, which is in the region bounded by the contour $\mathcal{C}$ and nearest to the point that $z=1$. If the generating function $P_{bb}(0;\xi)$ is divergent as $\xi\to 1^{-}$, the singular part of $P_{bb}(0;\xi)$ comes solely from the first term $P_{bb}^{(1)}(\xi)_{-}$ in equation (134). This is because, at $\xi=1$, $z_{-}^{(1)}(\xi)$ is the only pole on the unit circle, corresponding to the limit $E_1(0;1^{-})=1$ with $z_{-}^{(1)}=1$ and $k=0$. This fact will enormously simplify the study of the asymptotic behavior of the basic statistical properties for unbiased DRWs.

The physical meaning of the limit of the generating function $P_{bb}(0;\xi)$ as $\xi\to 1^{-}$, i.e., $P_{bb}(0;1^{-})=\displaystyle\sum_{n=0}^{\infty}P_{bb}(0)_n$, is the sum of the probability of return to the starting site over all possible step. The divergence of this sum implies that the event that the random walker returns to the starting site is certain to happen (see, e.g.,

subsection 2.3.3.). The divergent problem of this sum for a variety of random walk models has been extensively studied by many authors. It was first shown by Polya [57] that, for the symmetric Polya walk, the walk whose single-step transition probabilities to neighboring sites are equal, the sum is divergent if the dimension of the underlying lattice structure equals 1 or 2, while for higher dimensions the sum is convergent. This is the so-called Polya's theorem.

Since we are interested in quasi-1d infinite structures, in the sense of fractal dimensions, dimensions of quasi-1d infinite structures can be any real number between 1 to 2. There are several ways to define fractal dimensions. One of them is the so-called spectral dimension. The spectral dimension d_H is defined through the asymptotic form of the generating function $P_{bb}(0;\xi)$ of the probability of return to the starting site at certain steps (see Eq. 3.111 in [58]), i.e.,

$$P_{bb}(0;\xi) \sim \text{constant} \times (1-\xi)^{-(1-d_H/2)} \tag{135}$$

whose limit $P_{bb}(0;1^-)$ is divergent when $0 < d_H < 2$. Note that although there are many ways of defining fractal dimensions, these different ways are all related to each other. For quasi-1d infinite models, we notice that this parameter d_H is identical to the one introduced in the preceding subsection for many scenarios, so let us use the same notation for both parameters.

For our models, if the singularity $z_-^{(1)}(\xi)$ is a simple pole and the term $1-E_1(k(z);\xi)$ can be factorized as

$$1-E_1(k(z);\xi) = \frac{H(z;\xi)}{z}\left(z - z_-^{(1)}(\xi)\right) \tag{136}$$

where $H(z;\xi)$ is a certain function, and assume that the asymptotic form of the function $H(\xi) \equiv H\left(z_-^{(1)}(\xi);\xi\right)$ can be expressed as

$$H(\xi) \sim \frac{1}{c_2}(1-\xi)^{1-d_H/2} \tag{137}$$

where c_2 is a certain constant, then the first term of the generating function $P_{bb}(0;\xi)$ in equation (134) becomes

$$P_{bb}^{(1)}(\xi)_- = \frac{\text{adj}\left[\text{I-}\bar{\text{p}}\left(k\left(z_-^{(1)}(\xi)\right);\xi\right)\right]_{bb}}{\prod_{n=2}^{N_M}\left(1-E_n\left(k\left(z_-^{(1)}(\xi)\right);\xi\right)\right)} \frac{1}{H(\xi)}, \tag{138}$$

and its asymptotic form is the same as that shown in equation (135), i.e.,

$$P_{bb}(0;\xi) \sim c_2 \pi_b (1-\xi)^{-(1-d_H/2)} \tag{139}$$

where we have used relation (108).

Furthermore, from equations (106), (132) and (139), the asymptotic forms of the Laplace transform $P_{bb}^{*}(0,s)$ and the probability $P_{bb}(0,t)$ are $P_{bb}^{*}(0,s) \sim \frac{c_2 \pi_b}{s}(t_0 s)^{d_H v/2}$ and

$$P_{bb}(0,t) \sim \frac{c_2 \pi_b}{\Gamma\left(1-\frac{d_H v}{2}\right)}\left(\frac{t}{t_0}\right)^{-d_H v/2}. \tag{140}$$

It is worth pointing out that the exponent carries the important information of the underlying structure and the PDF of waiting time, i.e., the characteristic exponents d_H and v respectively. In addition, the analysis of $P_{ab}^{*}(0,s)$ and $P_{ab}(0;\xi)$ is analogous to that of $P_{bb}^{*}(0,s)$ and $P_{bb}(0;\xi)$. The only difference is $a \neq b$.

For quasi-1d infinite structure models, in the cases that the limit $P_{bb}(0;1^{-})$ of the generating functions $P_{bb}(0;\xi)$ are divergent, the restriction to the symmetric Polya walk may be dropped and replaced by unbiased DRWs. If DRW is unbiased along the structure axis, i.e., $\vartheta = 0$, it is likely to repeatedly visit the starting site. This leads to the divergence of the sum $P_{bb}(0;1^{-}) = \sum_{n=0}^{\infty} P_{bb}(0)_n$. In contrast, for biased DRWs, the sequence of the probabilities of return to the starting site decays rapidly and the sum is convergent. This can be verified in examples, but a general proof is lacking.

For biased DRWs, from equation (132), the asymptotic forms of the Laplace transform $P_{bb}^{*}(0,s)$ and the probability $P_{bb}(0,t)$ can be cast into the following forms: For $0 < v < 1$, $P_{bb}^{*}(0,s) \sim P_{bb}(0;1^{-}) t_0^{v} s^{v-1}$ and

$$P_{bb}(0,t) \sim \frac{P_{bb}(0;1^{-})}{\Gamma(1-v)}\left(\frac{t}{t_0}\right)^{-v}. \tag{141}$$

To sum up, the asymptotic behavior of the probability $P_{bb}(0,t)$ of return to the starting site at time t is determined by the asymptotic forms of the Laplace transform $\psi^{*}(s)$ of the PDF of waiting time and the generating function $P_{bb}(0;\xi)$ of the probability of return to the starting site at certain steps. The generating function

$P_{bb}(0;\xi)$ can be calculated from equation (133) in which the only information of the matrix $\bar{\mathrm{p}}(k;\xi)$ and certain relevant functions is required. We found that the probability $P_{bb}(0,t)$ behaves asymptotically in different regimes depending on the divergence of the generating function $P_{bb}(0;\xi)$ as $\xi \to 1^{-}$ which is governed by the localized transport of a walker and the geometrical characteristics of the underlying structure.

2.3.3 The probability of ever reaching a given major site

A random walk property closely related to the probability of return to the starting site is the probability of ever reaching a given major site. It can be obtained by realizing that if a walker has ever reached to that major site, it must visit the site for the first time at some times. Therefore, the probability $R_{ab}(m)$ of the walker ever reaching a given major site $\vec{x}_{m,a}$ is equal to the integral of the CFPP $F_{ab}(m,t)$ to that given site over all times,

$$R_{ab}(m) = \int_0^{\infty} F_{ab}(m,t)\,dt \tag{142}$$

which can also be calculated from the limit of the Laplace transform $F_{ab}^{*}(m,s)$,

$$R_{ab}(m) = \lim_{s\to 0^{+}} F_{ab}^{*}(m,s)\,. \tag{143}$$

To calculate this basic statistical property, let us employ equation (95). If the considered major site is the starting site, we have

$$F_{bb}^{*}(0,s) = 1 - \frac{1}{P_{bb}\left(0;\psi^{*}(s)\right)}\,. \tag{144}$$

As we discussed in the previous subsection, if the random walk is an unbiased DRW, the limit $P_{bb}(0;1^{-})$ is infinite, otherwise it is finite. From this statement and equations (143) and (144), they imply that the walker eventually reaches the starting site, i.e., $R_{bb}(0)=1$, if the walker is an unbiased DRW, otherwise, the event is not certain to happen, i.e., $R_{bb}(0)<1$.

This result coincides with the recurrence theorem (see Subsection 3.2.5 in [58]). In our terminology, the theorem states that if the major sites $\vec{x}_{m,a}$ and $\vec{x}_{0,b}$ are accessible from each other, that is, $R_{ab}(m)\neq 0$ and $R_{ba}(-m)\neq 0$, then either

$$R_{bb}(0) = R_{aa}(0) = R_{ba}(-m) = R_{ab}(m) = 1$$

or

$$R_{bb}(0)<1,\ R_{aa}(0)<1 \text{ and } R_{ba}(-m)R_{ab}(m)<1.$$

If the considered major site is not the starting site but still in the starting unit cell, from equation (95), we have

$$F_{ab}^{*}(0,s)=\frac{P_{ab}\left(0;\psi^{*}(s)\right)}{P_{aa}\left(0;\psi^{*}(s)\right)} \tag{145}$$

where $a\neq b$. From what we have learned, we can express this Laplace transform in the following form:

$$F_{ab}^{*}(0,s)=\frac{\sum_{i=1}^{I}P_{ab}^{(i)}\left(\psi^{*}(s)\right)_{-}}{\sum_{i=1}^{I}P_{aa}^{(i)}\left(\psi^{*}(s)\right)_{-}}. \tag{146}$$

It can be shown that $R_{ab}(0)=1$ for $a\neq b$ if the walk is an unbiased DRW and the term $E_1(k(z);\xi)$ satisfies equation (136). This is because the numerator in equation (146) is asymptotically equal to the denominator as $s\to 0^{+}$. However, if the walk is a biased DRW, in general, it is somewhat complicated to evaluate this probability because every term in the sums needs to be taken into account.

We have so far analyzed the probabilities for the sites contained in the starting unit cell, $m=0$, and we have known that the behavior of the poles $z_{-}^{(i)}(\xi)$ play an important role in determining the behavior of the probabilities. However, in general, the behavior of the poles may be different for $m\leq 0$ and $m>0$. Therefore, to distinguish them, let $z_{-}^{(i)}(\xi)$ and $z_{+}^{(i)}(\xi)$ denote the ith singularity for $m\leq 0$ and $m>0$ respectively.

Accordingly, for the major sites in the $m\neq 0$ unit cell, from equations (95) and (134), the expression of $F_{ab}^{*}(m,s)$ is analogous to equation (146) except for the additional terms and the additional subscripts,

$$F_{ab}^{*}(m,s)=\frac{\sum_{i=1}^{I}\left(z_{\pm}^{(i)}\left(\psi^{*}(s)\right)\right)^{|m|}P_{ab}^{(i)}\left(\psi^{*}(s)\right)_{\pm}}{\sum_{i=1}^{I}P_{aa}^{(i)}\left(\psi^{*}(s)\right)_{-}} \tag{147}$$

where the term $P_{ab}^{(i)}\left(\psi^{*}(s)\right)_{\pm}$ corresponds to the pole $z_{\pm}^{(i)}\left(\psi^{*}(s)\right)$.

For a board class of unbiased DRWs, models may have a reflective symmetry which leads to the identity $z_{+}^{(1)}\left(\psi^{*}(s)\right)=z_{-}^{(1)}\left(\psi^{*}(s)\right)$ and, of course, $P_{ab}^{(1)}\left(\psi^{*}(s)\right)_{+}=P_{ab}^{(1)}\left(\psi^{*}(s)\right)_{-}$. With the divergence of the limit $P_{ab}^{(1)}\left(1^{-}\right)_{-}$, the asymptotic form of the Laplace transform $F_{ab}^{*}(m,s)$ is

$$F_{ab}^{*}(m,s)\sim\left(z_{-}^{(1)}\left(\psi^{*}(s)\right)\right)^{|m|}. \tag{148}$$

Furthermore, from the definition, the pole $z_{-}^{(1)}\left(\psi^{*}(s)\right)$ approaches unity as $s\to 0^{+}$ so $R_{ab}(m)=1$ for $a,b=1,2,3,...,N_M$ and $m\neq 0$. If the walk is a biased DRW, it is obvious that the evaluation of the probability $R_{ab}(m)$ is more complicated than that of the cases $m=0$.

To summarize, for a board class of unbiased DRWs, it was found that every major sites on the structures are eventually reached by a random walker, i.e., $R_{ab}(m)=1$ for $a,b=1,2,3,...,N_M$ and any integer m, while, for biased DRWs, the evaluation of the probability $R_{ab}(m)$ is nontrivial because we need to know the exact values of the limit $z_{\pm}^{(i)}$ and the limit $P_{ab}^{(i)}\left(1^{-}\right)_{\pm}$.

2.3.4 The conditional mean first-passage time at a given major site

While the probability $R_{ab}(m)$ that a major site $\vec{x}_{m,a}$ is visited is one of the most important basic statistical properties of a random walk, it gives us only a rough picture of the temporal properties of the random walker. We can glean more information from the statistics of time on which the major site $\vec{x}_{m,a}$ first visited, that is, the first-passage time.

To avoid difficulties, we shall examine here the conditional mean first-passage time $\tau_{ab}(m)$ defined by

$$\tau_{ab}(m)\equiv\frac{1}{R_{ab}(m)}\int_{0}^{\infty}tF_{ab}(m,t)\,dt\,. \tag{149}$$

In words, the conditional mean first-passage time $\tau_{ab}(m)$ is the mean time that the random walker takes to visit a major site $\vec{x}_{m,a}$ for the first time, given that the walker initiated from the major site $\vec{x}_{0,b}$ and the major site $\vec{x}_{m,a}$ is eventually reached. From

this definition, it is straightforward that the conditional mean first-passage time $\tau_{ab}(m)$ can be calculated from

$$\tau_{ab}(m) = -\frac{1}{R_{ab}(m)} \lim_{s\to 0^+} \frac{\partial}{\partial s} F_{ab}\left(m;\psi^*(s)\right) \tag{150}$$

which gives

$$\tau_{ab}(m) = \tau_{ab}^{(D)}(m)\left(-\lim_{s\to 0^+} \frac{d}{ds}\psi^*(s)\right) \tag{151}$$

where

$$\tau_{ab}^{(D)}(m) \equiv \frac{1}{R_{ab}(m)} \lim_{\xi\to 1^-} \frac{\partial}{\partial \xi} F_{ab}(m;\xi) \tag{152}$$

is the conditional mean number of steps that the walker takes before visiting a given major site for the first time. Hence, the conditional mean first-passage time $\tau_{ab}(m)$ is the multiplication of the conditional mean number $\tau_{ab}^{(D)}(m)$ of steps and the mean time of the PDF of waiting time. This implies that the conditional mean first-passage time $\tau_{ab}(m)$ to a given major site is infinite if either one of these quantities is infinite.

If the walk is an unbiased DRW, the eigenfunction $E_1(k;\xi)$ satisfies equation (136), and the limits of the derivatives of the poles $z_{\pm}^{(1)}(\xi)$ as $\xi \to 1^-$ are infinite, i.e., for $1 \le d_H < 2$

$$\left(z_{\pm}^{(1)}(\xi)\right)' \sim c_3 (1-\xi)^{-d_H/2}, \tag{153}$$

then it can be shown that, for any major site $\vec{x}_{m,a}$, the conditional mean number $\tau_{ab}^{(D)}(m)$ of steps is infinite which leads to the infinite conditional mean first-passage time $\tau_{ab}(m)$.

To see this, let us recall the results in the previous subsection, for any major site $\vec{x}_{m,a}$, $R_{ab}(m) = 1$. Hence the calculation of the term $\tau_{ab}^{(D)}(m)$ is reduced to

$$\tau_{ab}^{(D)}(m) = \lim_{\xi\to 1^-} \frac{\partial}{\partial \xi} F_{ab}(m;\xi). \tag{154}$$

Therefore, what we need to do is to show that this limit is infinite.

For the starting major site, from equation (144), if the Laplace transform $\psi^*(s)$ is replaced by parameter ξ, we will obtain the simple relation between the generating functions $F_{bb}(0;\xi)$ and $P_{bb}(0;\xi)$,

$$F_{bb}(0;\xi) = 1 - \frac{1}{P_{bb}(0;\xi)}. \tag{155}$$

From this result and equation (139), we have

$$F_{bb}\left(0;\xi\right)\sim 1-\frac{1}{c_2\pi_b}\left(1-\xi\right)^{1-d_H/2}, \tag{156}$$

and

$$\frac{\partial}{\partial\xi}F_{bb}\left(0;\xi\right)\sim\frac{1-d_H/2}{c_2\pi_b}\left(1-\xi\right)^{-d_H/2} \tag{157}$$

is immediate. Therefore, $\lim_{\xi\to 1^-}\frac{\partial}{\partial\xi}F_{bb}\left(0;\xi\right)$ is infinite.

Similarly, for the other major sites in the starting unit cell, from equation (145), after employing the analogy of equation (138) and rearranging, we obtain

$$F_{ab}\left(0;\xi\right)=\frac{\dfrac{\mathrm{adj}\left[\mathrm{I}\text{-}\overline{\mathrm{p}}\left(k\left(z_-^{(1)}\right);\xi\right)\right]_{ab}}{\prod_{n=2}^{N_M}\left(1-E_n\left(k\left(z_-^{(1)}\right);\xi\right)\right)}+H\left(z_-^{(1)};\xi\right)\sum_{i>1}^{I}P_{ab}^{(i)}\left(\xi\right)_-}{\dfrac{\mathrm{adj}\left[\mathrm{I}\text{-}\overline{\mathrm{p}}\left(k\left(z_-^{(1)}\right);\xi\right)\right]_{aa}}{\prod_{n=2}^{N_M}\left(1-E_n\left(k\left(z_-^{(1)}\right);\xi\right)\right)}+H\left(z_-^{(1)};\xi\right)\sum_{i>1}^{I}P_{aa}^{(i)}\left(\xi\right)_-}. \tag{158}$$

To unclutter the notation, we have omitted the argument of the singularity $z_-^{(i)}\left(\xi\right)$. After differentiating this equation with respect to the parameter ξ, the asymptotic form of the result is obtained,

$$\frac{\partial}{\partial\xi}F_{ab}\left(0;\xi\right)\sim\left(\sum_{i>1}^{I}P_{aa}^{(i)}\left(1^-\right)_--\sum_{i>1}^{I}P_{ab}^{(i)}\left(1^-\right)_-\right)\left(\frac{1-d_H/2}{c_2\pi_a}\left(1-\xi\right)^{-d_H/2}\right) \tag{159}$$

and this is clear that its limit as $\xi\to 1^-$ is infinite. For the remaining major sites, from equation (148), we have

$$F_{ab}\left(m;\xi\right)\sim\left(z_\pm^{(1)}\left(\xi\right)\right)^{|m|}. \tag{160}$$

Then we differentiate this equation with respect to ξ and use the condition in equation (153). What we obtain is

$$\frac{\partial}{\partial\xi}F_{ab}\left(m;\xi\right)\sim c_3|m|\left(1-\xi\right)^{-d_H/2} \tag{161}$$

where $z_\pm^{(1)}=1$ was used. It is obvious that $\lim_{\xi\to 1^-}\frac{\partial}{\partial\xi}F_{ab}\left(m;\xi\right)=\infty$.

It is worth pointing out that, in many scenarios, e.g., unbiased DRWs, we notice that the conditional mean first-passage time $\tau_{ab}\left(m\right)$ to a given major site $\vec{x}_{m,a}$ is infinite but the event that the walker eventually reaches that major site is certain

to happen, i.e., $R_{ab}(m)=1$. This statement is not informative. However, we can consider the more informative temporal property, the conditional mean first-passage time $\tau_{ab}(m,t)$ to a given major site $\vec{x}_{m,a}$ by finite time t, given that the site is eventually visited by the time. It is defined by

$$\tau_{ab}(m,t)\equiv\frac{1}{R_{ab}(m,t)}\int_0^t t'F_{ab}(m,t')dt' \tag{162}$$

where $R_{ab}(m,t)\equiv\int_0^t F_{ab}(m,t')dt'$ is the probability that $\vec{x}_{m,a}$ is visited by time t.

To determine the asymptotic value of the conditional mean first-passage time $\tau_{ab}(m,t)$, let us examine the Laplace transform of an auxiliary function $Q_{ab}(m,t)\equiv\tau_{ab}(m,t)R_{ab}(m,t)$,

$$Q^*_{ab}(m,s)=\int_0^\infty \tau_{ab}(m,t)R_{ab}(m,t)e^{-st}dt\,. \tag{163}$$

We can rewrite this auxiliary Laplace transform in a more convenient form,

$$Q^*_{ab}(m,s)=-\frac{1}{s}\frac{d\psi^*(s)}{ds}\left.\frac{\partial F_{ab}(m;\xi)}{\partial\xi}\right|_{\xi=\psi^*(s)}. \tag{164}$$

It is obvious that this auxiliary function is of our interest because, for large time t, $\lim_{t\to\infty}R_{ab}(m,t)=R_{ab}(m)=1$, and $Q_{ab}(m,t)$ is asymptotically equal to $\tau_{ab}(m,t)$.

From equation (106), it can be easily shown that the asymptotic form of the Laplace transform $Q^*_{ab}(m,s)$ is determined by the asymptotic form of the first derivative of the generating function $F_{ab}(m;\xi)$,

$$Q^*_{ab}(m,s)\sim vt_0^v s^{v-2}\left.\frac{\partial F_{ab}(m;\xi)}{\partial\xi}\right|_{\xi=\psi^*(s)}, \tag{165}$$

which we have already considered.

If the walk is an unbiased DRW, the eigenfunction $E_1(k(z);\xi)$ satisfies equation (136), and the derivatives of the poles $z_\pm^{(1)}(\xi)$ as $\xi\to1^-$ are in the form shown in equation (153), then from equations (106), (157), (159), (161) and (165) we obtain the asymptotic behavior of the conditional mean first-passage time $\tau_{ab}(m,t)$,

$$\tau_{bb}(0,t)\sim\frac{vt_0(1-d_H/2)}{\Gamma\left(2-v(1-d_H/2)\right)c_2\pi_b}\left(\frac{t}{t_0}\right)^{1-v(1-d_H/2)}, \tag{166}$$

for the starting major site,

$$\tau_{ab}(0,t) \sim \left(\sum_{i>1}^{I} P_{aa}^{(i)}(1^-)_- - \sum_{i>1}^{I} P_{ab}^{(i)}(1^-)_- \right) \tau_{aa}(0,t), \quad (167)$$

for the other major sites in the starting unit cell,

$$\tau_{ab}(m,t) \sim \frac{c_3 v t_0 |m|}{\Gamma\left(2 - v\left(1 - d_H/2\right)\right)} \left(\frac{t}{t_0} \right)^{1 - v(1 - d_H/2)} \quad (168)$$

for the remaining major sites.

Summarizing, we found that the conditional mean first-passage time $\tau_{ab}(m)$ to a given major site $\vec{x}_{m,a}$ is equal to the multiplication of the conditional mean number $\tau_{ab}^{(D)}(m)$ of steps that a walker walks before visiting the given site for the first time and the mean time of the PDF of waiting time. In certain scenarios, the event that the walker ever reaches a given major site is certain to happen, i.e., $R_{ab}(m) = 1$, but we must wait for long time generally, i.e., $\tau_{ab}(m) = \infty$. The conditional mean first-passage time $\tau_{ab}(m)$ is thus no longer useful. However, we can consider the more useful temporal property, the conditional mean first-passage time $\tau_{ab}(m,t)$ to a given major site $\vec{x}_{m,a}$ by finite time t, given that the site is eventually visited by the time. To determine the asymptotic behavior of $\tau_{ab}(m,t)$ when time is large, the eigenfunction $E_1(k;\xi)$ and the derivatives of the poles $z_{\pm}^{(1)}(\xi)$ need to be satisfied several conditions.

2.3.5. The expected number of distinct major sites visited

In some contexts, we are also interested in the portion of the underlying structure explored by a walker. One of basic random walk properties which is related to this subject is the number of distinct sites visited at a certain time. In our model, the asymptotic behavior of the expected number $\langle S \rangle(t)$ of distinct major sites visited at time t can be determine by the concepts previously introduced.

To facilitate the analysis of $\langle S \rangle(t)$, let us introduce a new variable, $\langle \Delta \rangle(t)dt$, the expected number of new major sites visited at time t. By convention, the starting event is counted as a visit to the staring major site, so that we have

$$\langle \Delta \rangle(t) = \delta(t) + \sum_{\vec{x}_{m,a} \neq \vec{x}_{0,b}} F_{ab}(m,t), \quad (169)$$

and the corresponding Laplace transform is

$$\langle \Delta \rangle^{*}(s) = 1 - F_{bb}\left(0;\psi^{*}(s)\right) + \sum_{m=-\infty}^{\infty}\sum_{a=1}^{N_M} F_{ab}\left(m;\psi^{*}(s)\right). \tag{170}$$

Clearly, the expected number $\langle S \rangle(t)$ of distinct major sites visited at time t is identical to the integral of the expected number $\langle \Delta \rangle(t')$ of new major sites visited from the initial time $t'=0$ to the final time $t'=t$,

$$\langle S \rangle(t) = \int_0^t \langle \Delta \rangle(t')\,dt' \tag{171}$$

where its Laplace transform equals to

$$\langle S \rangle^{*}(s) = \frac{\langle \Delta \rangle^{*}(s)}{s}. \tag{172}$$

From the relation between the generating functions $F_{ab}\left(m;\psi^{*}(s)\right)$ and $P_{ab}\left(m;\psi^{*}(s)\right)$ in equation (95), we find that

$$\langle S \rangle^{*}(s) = \frac{1}{s}\sum_{m=-\infty}^{\infty}\sum_{a=1}^{N_M}\frac{P_{ab}\left(m;\psi^{*}(s)\right)}{P_{aa}\left(0;\psi^{*}(s)\right)}. \tag{173}$$

Since the sum $\sum_{m=-\infty}^{\infty} P_{ab}(m;\xi)$ equals to the Fourier transform $\bar{P}_{ab}(0;\xi)$ which is determined in equation (85), we can express the Laplace transform $\langle S \rangle^{*}(s)$ as

$$\langle S \rangle^{*}(s) = \frac{1}{s}\frac{1}{\left(1-E_1\left(0;\psi^{*}(s)\right)\right)}\sum_{a=1}^{N_M}\frac{\mathrm{adj}\left[\mathrm{I}-\bar{\mathrm{p}}\left(0;\psi^{*}(s)\right)\right]_{ab}}{\prod_{n=2}^{N_M}\left(1-E_n\left(0;\psi^{*}(s)\right)\right)}\frac{1}{P_{aa}\left(0;\psi^{*}(s)\right)}. \tag{174}$$

If the random walk is a DRW, the asymptotic form of $\langle S \rangle^{*}(s)$ becomes

$$\langle S \rangle^{*}(s) \sim \frac{1}{c_1 s\left(t_0 s\right)^{\nu(2-d_H)}}\sum_{a=1}^{N_M}\frac{\pi_a}{P_{aa}\left(0;\psi^{*}(s)\right)}. \tag{175}$$

Recall that, for unbiased DRWs with $E_1\left(0;\psi^{*}(s)\right)$ obeying equation (136), $P_{aa}\left(0;\psi^{*}(s)\right)$ is determined by equation (139), and we can verify immediately that

$$\langle S \rangle^{*}(s) \sim \frac{1}{s}\frac{N_M}{c_1 c_2}\left(t_0 s\right)^{-\frac{\nu}{2}(2-d_H)}, \tag{176}$$

$$\langle S \rangle(t) \sim \frac{1}{\Gamma\left(1+\frac{\nu}{2}(2-d_H)\right)}\frac{N_M}{c_1 c_2}\left(\frac{t}{t_0}\right)^{\frac{\nu}{2}(2-d_H)}. \tag{177}$$

For biased DRWs, in equation (175), there is no divergent term in the sum so

$$\langle S\rangle(t) \sim \frac{\sum_{a=1}^{N_M} \frac{\pi_a}{P_{aa}\left(0;1^-\right)}}{\Gamma\left(1+v\left(2-d_H\right)\right)c_1}\left(\frac{t}{t_0}\right)^{v(2-d_H)} . \tag{178}$$

From this result, to completely determine the asymptotic behavior of the expected number $\langle S\rangle(t)$, we need to take into account all values of the limits $P_{aa}\left(0;1^-\right)$ for $a=1,2,3,...,N_M$.

In summary, after determining the important quantities, e.g., c_1, c_2, π_a and $P_{aa}\left(0;1^-\right)$, the asymptotic form of the expected number of distinct major sites visited at time t can be calculated from

$$\langle S\rangle(t) \sim \begin{cases} \dfrac{1}{\Gamma\left(1+\dfrac{v}{2}\left(2-d_H\right)\right)}\dfrac{N_M}{c_1c_2}\left(\dfrac{t}{t_0}\right)^{\frac{v}{2}(2-d_H)} & ;\vartheta=0 \\ \dfrac{\sum_{a=1}^{N_M}\dfrac{\pi_a}{P_{aa}\left(0;1^-\right)}}{\Gamma\left(1+v\left(2-d_H\right)\right)c_1}\left(\dfrac{t}{t_0}\right)^{v(2-d_H)} & ;\vartheta\neq 0 \end{cases} . \tag{179}$$

2.4 Summary

Our main result of this chapter is the prescription which can be used to obtain the asymptotic behavior of the basic statistical properties of the random walk on a quasi-1d infinite structure. The following table summarizes the main steps in the prescription.

I. Determine the Fourier transform $\bar{\mathrm{p}}\left(k;\xi\right)$ of the generating function of the transition probability matrix. It is defined by

$$\bar{\mathrm{p}}\left(k;\xi\right) \equiv \begin{bmatrix} \bar{p}_{11}\left(k;\xi\right) & \cdots & \bar{p}_{1N_M}\left(k;\xi\right) \\ \vdots & \ddots & \vdots \\ \bar{p}_{N_M1}\left(k;\xi\right) & \cdots & \bar{p}_{N_MN_M}\left(k;\xi\right) \end{bmatrix} \tag{180}$$

where $\bar{p}_{ab}\left(k;\xi\right) \equiv \sum_{\Delta m=-1}^{1} e^{ik\Delta mL}\left(\sum_{n=0}^{\infty} p_{ab}\left(\Delta m\right)_n \xi^n\right)$. The term $p_{ab}\left(\Delta m\right)_n$ is the n-step transition probability from a major site $\vec{x}_{0,b}$ to a given major site $\vec{x}_{\Delta m,a}$, given that the walker does not visit any major site during the transition.

II. Find the eigenfunction $E_1(k;\xi)$ and the limit $\pi \equiv \lim_{\xi\to 1^-}\pi(0;\xi)$ of the corresponding eigenvector $\pi(k;\xi)$ of the matrix $\bar{\mathrm{p}}(k;\xi)$.

III. Extract the parameters c_1 and d_H from the asymptotic form

$$1-E_1(0;\xi)\sim c_1(1-\xi)^{2-d_H}. \tag{181}$$

IV. Calculate the effective velocity $\mathcal{G}$ and the diffusion coefficient D from

$$\mathcal{G}=\frac{1}{\Gamma\left(1+\nu\left(2-d_H\right)\right)c_1t_0^{\nu(2-d_H)}}\sum_{a,b=1}^{N_M}\left(\frac{\partial}{i\partial k}\bar{p}_{ab}\left(k;1^-\right)\Big|_{k=0}\right)\pi_b \tag{182}$$

where $\Gamma(z)$ is the gamma function and

$$D=\frac{1}{2\Gamma\left(1+\nu\left(2-d_H\right)\right)c_1t_0^{\nu(2-d_H)}}\sum_{a,b=1}^{N_M}\left(\frac{\partial^2}{i^2\partial k^2}\bar{p}_{ab}\left(k;1^-\right)\Big|_{k=0}\right)\pi_b. \tag{183}$$

The asymptotic form of the first and the second moment are

$$\langle x\rangle(t)\sim \mathcal{G}t^{\nu(2-d_H)}, \tag{184}$$

$$\left\langle x^2\right\rangle(t)\sim\frac{2\Gamma^2\left(1+\nu\left(2-d_H\right)\right)}{\Gamma\left(1+2\nu\left(2-d_H\right)\right)}\langle x\rangle^2(t)+2Dt^{\nu(2-d_H)}. \tag{185}$$

V. Determine the generating function $\mathrm{P}(m;\xi)$ whose entries can be calculated from

$$P_{ab}(m;\xi)=\frac{1}{2\pi i}\oint_{\mathcal{C}}\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(k(z);\xi\right)\right]^{-1}_{ab}z^{-m}\frac{dz}{z} \tag{186}$$

where $a,b=1,2,3,\ldots,N_M$, m is an integer and the contour $\mathcal{C}$ is the unit circle. The resulting expression of $P_{ab}(m;\xi)$ may be in the form

$$P_{ab}(m;\xi)=\sum_{i=1}^{I}\left(z_{\pm}^{(i)}(\xi)\right)^{|m|}P_{ab}^{(i)}(\xi)_{\pm}. \tag{187}$$

For $m\le 0$, the term $z_{-}^{(i)}(\xi)$ is the pole of $\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(k(z);\xi\right)\right]^{-1}_{ab}$ which is in the region bounded by the contour $\mathcal{C}$, and $P_{ab}^{(i)}(\xi)_{-}$ is the certain function associated with this pole. For $m>0$, the term $z_{+}^{(i)}(\xi)$ is the pole of the term $\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(k(z);\xi\right)\right]^{-1}_{ab}$ for the modified coordinate, the coordinate corresponding to the unit vector $\hat{x}$ flipped.

VI. For DRWs biased along the structure axis, i.e., $\mathcal{G}\neq 0$, the explicit form of the generating function $P_{ab}(m;\xi)$ is desired, and the asymptotic behavior of the random walk properties can be determined as the following;

the probability $P_{bb}(0,t)$ of return to the starting site $\vec{x}_{0,b}$ at large times,

$$P_{bb}(0,t) \sim \frac{P_{bb}(0;1^-)}{\Gamma(1-\nu)}\left(\frac{t}{t_0}\right)^{-\nu} \text{ for } 0<\nu<1, \tag{188}$$

the probability $R_{ab}(m)$ of ever reach a given major site $\vec{x}_{m,a}$,

$$R_{ab}(m) = \lim_{\xi\to 1^-} \frac{P_{ab}(m;\xi) - \delta_{m,0}\delta_{a,b}}{P_{aa}(0;\xi)}, \tag{189}$$

the conditional mean first-passage time $\tau_{ab}(m)$ to a given major site $\vec{x}_{m,a}$,

$$\tau_{ab}(m) = \frac{1}{R_{ab}(m)} \lim_{\xi\to 1^-} \frac{\partial}{\partial \xi}\left\{\frac{P_{ab}(m;\xi) - \delta_{m,0}\delta_{a,b}}{P_{aa}(0;\xi)}\right\} t_0 \text{ for } \nu=1 \tag{190}$$

and the expected number $\langle S\rangle(t)$ of distinct major sites visited at large times,

$$\langle S\rangle(t) \sim \frac{\sum_{a=1}^{N_M} \frac{\pi_a}{P_{aa}(0;1^-)}}{\Gamma(1+\nu(2-d_H))c_1}\left(\frac{t}{t_0}\right)^{\nu(2-d_H)}. \tag{191}$$

VII. However, for DRWs unbiased along the structure axis, i.e., $\vartheta = 0$, the asymptotic forms of the singular part of the generating function $P_{bb}(0;\xi)$ is sufficient to determine the asymptotic behavior of the random walk properties. In particular, we need to extract the parameters c_2 and c_3 from the asymptotic forms of $P_{bb}^{(1)}(\xi)_-$ and $\left(z_-^{(1)}(\xi)\right)'$ respectively,

$$P_{bb}^{(1)}(\xi) \sim \pi_b c_2 (1-\xi)^{-(1-d_H/2)}, \tag{192}$$

$$\left(z_-^{(1)}(\xi)\right)' \sim c_3 (1-\xi)^{-d_H/2}. \tag{193}$$

Then the random walk properties are

the probability of return to the starting site at large times,

$$P_{bb}(0,t) \sim \frac{c_2\pi_b}{\Gamma\left(1-\frac{d_H\nu}{2}\right)}\left(\frac{t}{t_0}\right)^{-d_H\nu/2}, \text{ for } 0<\nu\le 1, \tag{194}$$

the probability of ever reach any major site is unity, $R_{ab}(m)=1$,

the conditional mean first-passage time to any major site is infinite, $\tau_{ab}(m)=\infty$,

the conditional mean first-passage time to a given major site by large times,

for the starting major site,

$$\tau_{bb}(0,t) \sim \frac{\nu t_0(1-d_H/2)}{\Gamma(2-\nu(1-d_H/2))c_2\pi_b}\left(\frac{t}{t_0}\right)^{1-\nu(1-d_H/2)}, \tag{195}$$

for the other major sites in the starting unit cell,

$$\tau_{ab}(0,t) \sim \left(\sum_{i \neq 1} P_{aa}^{(i)} - \sum_{i \neq 1} P_{ab}^{(i)} \right) \tau_{aa}(0,t), \tag{196}$$

and, for the remaining major sites,

$$\tau_{ab}(m,t) \sim \frac{c_3 v t_0 |m|}{\Gamma\left(2 - v\left(1 - d_H/2\right)\right)} \left(\frac{t}{t_0} \right)^{1 - v(1 - d_H/2)}, \tag{197}$$

and the expected number of distinct major sites visited at large times,

$$\langle S \rangle(t) \sim \frac{1}{\Gamma\left(1 + v d_H/2\right)} \frac{N_M}{c_1 c_2} \left(\frac{t}{t_0} \right)^{\frac{v}{2}(2 - d_H)}. \tag{198}$$

The above equations, which will allow us to deduce many basic statistical properties of a random walk from equations (180) and (186) for the matrix $\bar{\mathrm{p}}(k;\xi)$ and the generating function $P_{ab}(m;\xi)$ respectively, are general but quite formal. In fact, the reader may feel that these relations are rather useless since, in general, the multi-step transition probabilities $p_{ab}(\Delta m)_n$ and the integral (186) must be expected to be very difficult to calculate for a random walk with a complex structure. While such an attitude is perhaps justified in complicated cases, there are many models for which considerable progress of one kind or another can be made. The rest of this thesis will be devoted to such examples.

3

Random walks on an unrestricted 1-d lattice

This chapter is devoted to considering the simplest case of a random walk on quasi-1d infinite structures, a random walk on a perfect 1-d lattice or an unrestricted 1-d lattice, which is discussed in most books on statistics or statistical physics (see, e.g., [59, 60]). The purpose we will consider this model in a bit more detail is twofold: to demonstrate the use of the generating function formalism developed in the previous chapter, and to verify our results with the well-known results to check if the formalism works as expected.

3.1 Model

For an unrestricted 1-d lattice, there are many choices of the site partition. For sake of simplicity, let us choose the simplest choice, each unit cell of the unrestricted 1-d lattice containing only one major site, i.e., $N = N_M = 1$. Hence there are not minor sites. It is assumed that a walker takes instantaneous step from one major site to the left and the right neighboring major sites or itself with single-step transition probabilities γ, α, and β, respectively (see Figure 17).

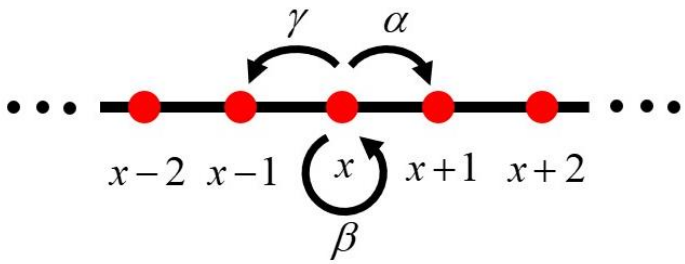


Figure 17. A schematic representation of the possible steps of a walker with the corresponding single-step transition probabilities.

Accordingly, the transition probability $p_{11}(\Delta m)_n$ that the walker takes steps from a major site to the nearest major sites can be written as

$$p_{11}(\Delta m)_n = \left(\gamma\delta_{\Delta m,-1} + \beta\delta_{\Delta m,0} + \alpha\delta_{\Delta m,1}\right)\delta_{n,1} \tag{199}$$

with $\gamma+\beta+\alpha=1$. In addition, between successive steps, the walker waits for a random time distributed according to a probability distribution function with finite mean, i.e., $\nu=1$ and $t_0<\infty$.

3.2 Results and discussion

As we have learned, GFF for obtaining the asymptotic behavior of the basic random walk properties is based on the information of the matrix $\overline{\mathrm{p}}(k;\xi)$ and the relevant functions. For the unrestricted 1-d lattice model, from equation (199), it is straightforward that

$$\overline{\mathrm{p}}(k;\xi) = \xi\left(\gamma e^{-iLk} + \beta + \alpha e^{iLk}\right). \tag{200}$$

One of the important relevant functions is the eigenfunction $E_1(k;\xi)$ which plays a crucial role in governing the asymptotic behavior of the basic properties. Since, in this case, the matrix $\overline{\mathrm{p}}(k;\xi)$ is a 1×1 matrix, there is only one eigenvector $\pi(k;\xi)=1$ with the corresponding eigenfunction

$$E_1(k;\xi) = \overline{\mathrm{p}}(k;\xi). \tag{201}$$

This coincides with our intuition that the event that the walker is at a major site at large steps is certain to happen, i.e., $\pi_1=1$, and the random walk is a DRW, i.e., $E_1(0;1^-)=1$.

As shown in Subsection 2.3.1, the parameters c_1 and d_H, which are defined by the asymptotic form of $1-E_1(0;\xi)$, govern how the first and the second moments of the walker location along the structure axis asymptotically evolve with time. From equations (200) and (201), we have

$$1-E_1(0;\xi)=1-\xi \tag{202}$$

which gives

$$c_1=1 \text{ and } d_H=1. \tag{203}$$

Putting these parameters into equations (182) and (183) yields the effective velocity and the diffusion coefficient. We find that the effective velocity is equal to the "speed" of the walker, L/t_0, timed the degree of bias, $\alpha-\gamma$, i.e.,

$$\vartheta=(\alpha-\gamma)\frac{L}{t_0}. \tag{204}$$

It is obvious that the identity $\alpha=\gamma$ implies vanishing of the effective velocity which is the characteristic of an unbiased random walk. For the diffusion coefficient, we find that it equals to the single-step transition probability α timed the scaling variable $L/t_0^{1/2}$ squared,

$$D=\alpha\frac{L^2}{t_0}. \tag{205}$$

As these essential variables are determined, the first and the second moments are immediate,

$$\langle x\rangle(t)\sim\vartheta t \tag{206}$$

and

$$\langle x^2\rangle(t)\sim\langle x\rangle^2(t)+2Dt. \tag{207}$$

From the resulting first moment, when the walker is biased in either direction, regardless of the motion fluctuation, its averaged motion is like the ballistic motion with a constant velocity ϑ, the distance is proportional to time. For the second moment, if the random walk is unbiased, the second moment is proportional to time. This implies that the transport process is the so-called normal diffusion.

To determine the asymptotic behavior of the other basic properties, the matrix generating function $\mathrm{P}(m;\xi)$ is required. For this simplest random walk model, this matrix is a 1×1 matrix, i.e., $\mathrm{P}(m;\xi)=P_{11}(m;\xi)$, and the explicit form of the generating function $P_{11}(m;\xi)$ of the probability $P_{11}(m)_n$ that the walker is found at a major site $\vec{x}_{m,1}$ at certain step n is not hard to be calculated. Let us consider equation (186) for this model,

$$P_{11}(m;\xi)=-\frac{1}{\alpha\xi}\times\frac{1}{2\pi i}\oint_C\left(z^2-\left(\frac{1}{\alpha\xi}-\frac{\beta}{\alpha}\right)z-\frac{\gamma}{\alpha}\right)^{-1}z^{-m}dz \tag{208}$$

where $z\equiv e^{iLk}$ and we have used

$$\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(k(z);\xi\right)\right]^{-1}=\left(1-\xi\left(\gamma\frac{1}{z}+\beta+\alpha z\right)\right)^{-1}. \tag{209}$$

The resulting generating function is (see Appendix 8)

$$P_{11}(m;\xi)=P_{11}^{(1)}(\xi)_{\pm}\times\begin{cases}\left(z_{+}^{(1)}(\xi)\right)^{|m|};m>0\\ \left(z_{-}^{(1)}(\xi)\right)^{|m|};m\le 0\end{cases} \tag{210}$$

where

$$P_{11}^{(1)}(\xi)_{+}=P_{11}^{(1)}(\xi)_{-}=\frac{1}{H(\xi)}=\frac{1}{\sqrt{(1-\beta\xi)^2-4\alpha\gamma\xi^2}},$$

$$z_{-}^{(1)}(\xi)=\frac{1}{2\alpha\xi}\left((1-\beta\xi)-\sqrt{(1-\beta\xi)^2-4\alpha\gamma\xi^2}\right),$$

$$z_{+}^{(1)}(\xi)=\frac{1}{2\gamma\xi}\left((1-\beta\xi)-\sqrt{(1-\beta\xi)^2-4\alpha\gamma\xi^2}\right).$$

For the unbiased DRWs, $\alpha=\gamma$, we have developed the formulae, which are required only two parameters c_2 and c_3 determined by the asymptotic forms of the functions $P_{11}^{(1)}(\xi)_{\pm}$ and $z_{\pm}^{(1)}(\xi)$, respectively, to determine the asymptotic behavior of the certain basic properties. From the preceding results together with equations (192) and (193), we have

$$c_2=c_3=\frac{1}{2\sqrt{\alpha}}. \tag{211}$$

Putting the resulting parameter c_2 into equation (194) gives us the asymptotic form of the probability of return to the starting site for the unbiased random walks,

$$P_{11}(0,t)\sim\frac{1}{2\sqrt{\pi\alpha}}\left(\frac{t}{t_0}\right)^{-1/2}. \tag{212}$$

This is the well-known result and coincides with the scaling collapse in equation (7).

To obtain the probability $R_{11}(m)$ of ever reach a given major site $\vec{x}_{m,1}$ for general cases, i.e., biased and unbiased random walks, we need to know the values of the limit $P_{11}(m;1^{-})$ for any integer m. According to equation (210), it is

$$P_{11}(m;1^{-})=\frac{\left(\frac{1}{2}\left(|\alpha+\gamma|-|\alpha-\gamma|\right)\right)^{|m|}}{|\alpha-\gamma|}\times\begin{cases}\gamma^{-|m|};m>0\\ \alpha^{-|m|};m\le 0\end{cases}. \tag{213}$$

This resulting limit together with equation (189), we obtain

$$R_{11}(0)=\begin{cases}1-|\alpha-\gamma| & ;\alpha\neq\gamma\\ 1 & ;\alpha=\gamma\end{cases}, \tag{214}$$

$$R_{11}(m>0)=\begin{cases}1 & ;\alpha\geq\gamma\\ (\alpha/\gamma)^{m} & ;\alpha\leq\gamma\end{cases}, \tag{215}$$

$$R_{11}(m<0)=\begin{cases}(\gamma/\alpha)^{|m|} & ;\alpha\geq\gamma\\ 1 & ;\alpha\leq\gamma\end{cases}. \tag{216}$$

As we can see, when the random walk is unbiased, $\alpha=\gamma$, every site on the structure is eventually reached by the walker, i.e., $R_{11}(m)=1$ for any integer m. In contrast, for the biased random walks, $\alpha\neq\gamma$, if the considered major site is located in the same direction of bias, e.g., $m>0$ and $\alpha>\gamma$, the event of reaching that site is certain to happen. If the considered major site is located in the opposite direction of bias, e.g., $m<0$ and $\alpha>\gamma$, the probability of reaching that site decreases exponentially as the distance from the starting site increases.

Unlike the preceding basic property, to express the explicit form of the conditional mean first-passage time to a given major site, the values of the limit $\left(P_{11}(m;1^{-})\right)'$ for any integer m are essential. From equations (190) and (210), it is not difficult to show that

$$\tau_{11}(m)=\left|\frac{L}{\vartheta}\right|\times\begin{cases}\dfrac{|\alpha+\gamma|-|\alpha-\gamma|^{2}}{1-|\alpha-\gamma|} & ;m=0\\ |m| & ;m\neq 0\end{cases} \tag{217}$$

where we have used $\left(\dfrac{P_{11}(m;1^{-})}{P_{11}(0;1^{-})}\right)'=\dfrac{|m|R_{11}(m)}{|\alpha-\gamma|}$ and $-\left(\dfrac{1}{P_{11}(0;1^{-})}\right)'=\left|\dfrac{\alpha+\gamma}{\alpha-\gamma}\right|+|\alpha-\gamma|$.

Note that, in the limit that the random walk is unbiased, i.e., $\vartheta=0$, the conditional mean first-passage time to any major site is infinite. Vice versa, $\tau_{11}(m)$ is finite and equal to the absolute value of the distance, Lm, divided by the effective velocity, ϑ, if $m\neq 0$. However, in the case of $\vartheta=0$, if the arrival of the walker to a certain major site by a certain time is of interest, the conditional mean first-passage time to a given major site by a certain time is more informative than the above and can be obtain by substituting the parameter $c_2=c_3=1/\left(2\sqrt{\alpha}\right)$ into equations (195) and (197). After substituting, we will obtain

$$\tau_{11}(m,t) \sim \frac{t_0}{\sqrt{\pi}}\left(\frac{t}{t_0}\right)^{\frac{1}{2}} \times \begin{cases} 2\sqrt{Dt_0}/L & ;m=0 \\ |m|L/\sqrt{Dt_0} & ;m\neq 0 \end{cases} \tag{218}$$

where the relation $\alpha = Dt_0/L^2$ has been used. Although, it is intuitive that the conditional mean time $\tau_{11}(m,t)$ to the starting site (other sites) increases (decreases) as the diffusivity increases, interestingly, it is not proportional to the diffusivity but the square root of it.

Finally, we have had all important quantities including $P_{aa}(0;\xi)$, N_M, π_a, c_1, c_2, ν and d_H for calculating the asymptotic behavior of the expected number of distinct major sites visited at large times. After plugging them into equations (191) and (198), we obtain

$$\langle S\rangle(t) \sim \begin{cases} \frac{4}{L}\sqrt{\frac{Dt_0}{\pi}}\left(\frac{t}{t_0}\right)^{\frac{1}{2}} & ;\vartheta = 0 \\ \frac{\vartheta}{L}t & ;\vartheta \neq 0 \end{cases}. \tag{219}$$

Interestingly, at large times, for the biased random walks, the ratio of $\langle S\rangle(t)L$ and $\sqrt{\langle x^2\rangle(t)}$ is unity, while, for the unbiased random walks, this ration is not unity but $\sqrt{8/\pi}$. This is true independent of the details of the localized transition, i.e., the values of α, γ and β.

In summary, we have shown that the well-known basic properties of the random walks on an unrestricted 1-d lattice (see, e.g., [1, 38, 58, 61]) could be found by GFF. For examples, for the unbiased random walks, (i) the second moment of the random walk location along the structure axis at large times is proportional to time, (ii) the probability of return to the starting site at large times is a power function of time with exponent $-1/2$, and (iii) every site on the structure is eventually reached. To demonstrate the wide range of abilities of GFF, in the next chapter, it will be applied GFF to more complicated models, random walks on branched structures.

4

Random walks on branched lattices

As our second specific application of the GFF, we consider random walks on branched lattices. A schematic of this kind of structures is shown in Figure 18. At the outset, we treat the basic statistical properties of general cases in which the details of connected lattice networks and localized transport of a walker are not specified. This treatment will be applied to the study of the basic properties of the so-called comb model and its generalization.

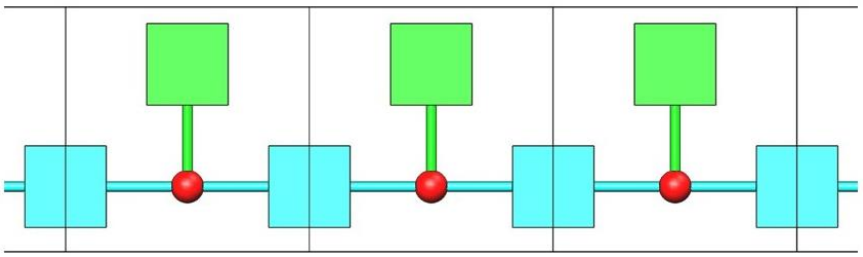


Figure 18. A schematic of the structure of the branched lattice. In each unit cell, there exist two lattice networks represented in blue and green boxes respectively, which are connected to each other by a major site represented in a red sphere.

4.1 Model

Here, a branched lattice is defined as a lattice system consists of periodically repeated unit cells connecting to each other in a one-dimensional fashion. A schematic of this kind of structures is shown in Figure 18. In each unit cell, there exists one major site (a red sphere) which is connected to its equivalent site in the next unit cell by a lattice network A (a blue box). The line passing through all major sites is called the structure axis or the backbone. There may be a dangling lattice network B (a green box) attached to each major site. It is assumed that the

networks A and B consist of N_{A} and N_{B} different minor sites, respectively. Thus, each unit cell contains $N = N_{\mathrm{A}} + N_{\mathrm{B}} + 1$ different sites. Figure 19 shows certain possibilities of branched lattices.

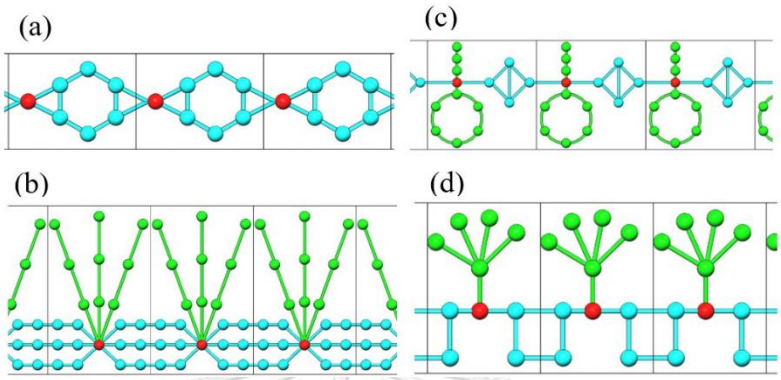


Figure 19. Unit cells of four different branched lattices.

Here, we will use the same coordinate system established in Chapter 2. Hence, the position of the major site in the m th unit cell indicated by the vector $\vec{x}_{m,1} = mL\hat{x} + \vec{r}_1$ with $\vec{r}_1 = 0$, and the position of the a th minor site in the m th unit cell indicated by the vector $\vec{x}_{m,a} = mL\hat{x} + \vec{r}_a$ where $a = 2, 3, ..., N$. Figure 20 illustrates the arrows representing certain vectors of lattice (b) in Figure 19.

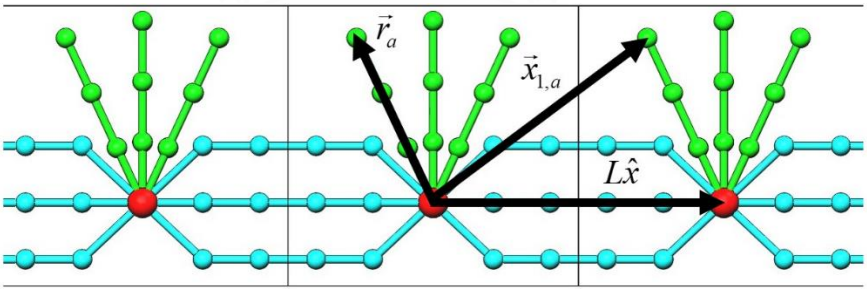


Figure 20. The arrows representing certain vectors of lattice (b) in Figure 19.

4.2 General cases

Let us develop general formulation which relates the basic random walk properties to a single function,

$$\overline{\mathrm{p}}(k;\xi) \equiv \sum_{\Delta m=-1}^{1} \left(\sum_{n=0}^{\infty} p_{11}(\Delta m)_n \, \xi^n \right) e^{iLk\Delta m} \tag{220}$$

where $p_{11}(\Delta m)_n$ is the n-step transition probability of steps from a major site $\vec{x}_{0,1}$ to a major site $\vec{x}_{\Delta m,1}$. From the restrictions of the walker stepping and the geometrical characteristics of the underlying structures (see Figure 18), we can write $p_{11}(0)_n = \alpha F(0|\alpha)_{n-1} + \gamma F(0|\gamma)_{n-1} + \beta F(0|\beta)_{n-1}$, $p_{11}(1)_n = \alpha F(1|\alpha)_{n-1}$ and $p_{11}(-1)_n = \gamma F(-1|\gamma)_{n-1}$ where α, γ, β are the single-step transition probabilities that the walker at a major site enters the right, the left and the up connected lattice networks respectively, given that $\alpha + \gamma + \beta = 1$. In turn, $F(1|\alpha)_n$, $F(-1|\gamma)_n$ and $F(0|\bullet)_n$ are respectively the conditional n-step transition probabilities that, after entering the connected lattice networks, the walker reaches the right, the left nearest major sites and the commencing major site itself for the first time without visiting other major sites. Substituting these expressions into equation (220) yields

$$\overline{\mathrm{p}}(k;\xi) = \Sigma(\xi) + \alpha^*(\xi)e^{iLk} + \gamma^*(\xi)e^{-iLk} \tag{221}$$

where $\Sigma(\xi) \equiv \alpha\xi F(0;\xi|\alpha) + \gamma\xi F(0;\xi|\gamma) + \beta\xi F(0;\xi|\beta)$, $\alpha^*(\xi) \equiv \alpha\xi F(1;\xi|\alpha)$ and $\gamma^*(\xi) \equiv \gamma\xi F(-1;\xi|\gamma)$. We now assume that when the walker enters the lattice networks linked two nearest major sites, it will spend finite time and will not get lost in the networks so that $(\alpha^*)' + (\gamma^*)' < \infty$, $F(1;1^-|\alpha) + F(0;1^-|\alpha) = 1$ and $F(-1;1^-|\gamma) + F(0;1^-|\gamma) = 1$. However, it may spend infinite time and may get lost in the dangling network, i.e., $(\Sigma)' \le \infty$ and $F(0;1^-|\beta) \le 1$.

Since this is the one-major-site problem, the primary results are analogous to that of the random walk on an unrestricted 1-d lattice, i.e., $E(k;\xi) = \overline{\mathrm{p}}(k;\xi)$ or

$$E(k;\xi) = \Sigma(\xi) + \alpha^*(\xi)e^{iLk} + \gamma^*(\xi)e^{-iLk} \tag{222}$$

and $\pi(k;\xi) = 1$. If each connected lattice network has a finite size, then the random walk is a DRWFG,

$$1 - E(0;\xi) \sim G(1-\xi), \tag{223}$$

which give

$$c_1 = G \text{ and } d_H = 1, \tag{224}$$

where G can be calculated from the given generating function $\Sigma(\xi)$, $\alpha^*(\xi)$ and $\gamma^*(\xi)$, i.e., $G = (\Sigma)' + (\alpha^*)' + (\gamma^*)'$.

From the resulting parameters together with equations (182) and (183), we have

$$\mathcal{G} = \frac{L\left(\alpha^* - \gamma^*\right)}{\Gamma\left(1+\nu\right) G t_0^{\nu}} \tag{225}$$

and

$$D = \frac{\alpha^* L^2}{\Gamma\left(1+\nu\right) G t_0^{\nu}}. \tag{226}$$

It may be noticed that an unrestricted 1-d lattice model is a special case of a branched lattice model. For the random walk on an unrestricted 1-d lattice, the average number of steps taken in connected lattice networks is zero, $G = 1$, because there is not a minor site. The multi-step transition probabilities α^* and γ^* are reduced to the single-step transition probabilities α and γ, and the PDF of waiting time is assumed to have the first moment, $\nu = 1$.

According to the preceding results, the first two moments are immediate,

$$\left\langle x \right\rangle\left(t\right) \sim \mathcal{G} t^{\nu} \tag{227}$$

and

$$\left\langle x^2 \right\rangle\left(t\right) \sim \frac{2\Gamma^2\left(1+\nu\right)}{\Gamma\left(1+2\nu\right)} \left\langle x \right\rangle^2\left(t\right) + 2Dt^{\nu}. \tag{228}$$

As you can see, the random walk can display normal diffusion and subdiffusion, which is dependent on the characteristic exponent of the PDF of waiting time.

On the other hand, for infinite-size dangling networks, these results are not always appliable. To see this, let us concentrate on the dangling networks as fractals with the spectral dimension $0 < d_H' < 2$, i.e., the generating function $P\left(0;\xi\middle|\beta\right)$ of the corresponding probability of return to the starting site, which is the commencing major site, obeys the equation $P\left(0;\xi\middle|\beta\right) \sim c_0\left(1-\xi\right)^{-\left(1-d_H'/2\right)}$. To proceed with the analysis, we rewrite equation (222) as

$$\begin{aligned} 1 - E\left(0;\xi\right) = \; & \left(\alpha+\gamma+\beta\right) - \left(\alpha\xi F\left(0;\xi\middle|\alpha\right) + \gamma\xi F\left(0;\xi\middle|\gamma\right) + \beta\xi F\left(0;\xi\middle|\beta\right)\right) \\ & - \alpha\xi F\left(1;\xi\middle|\alpha\right) - \gamma\xi F\left(-1;\xi\middle|\gamma\right) \end{aligned}. \tag{229}$$

Then, from the proposed assumption, we find

$$1 - E\left(0;\xi\right) \sim \beta\left(1 - F\left(0;\xi\middle|\beta\right)\right). \tag{230}$$

From the analogy of relation (92), $F\left(0;\xi|\beta\right)=1-\left[P\left(0;\xi|\beta\right)\right]^{-1}$, we finally obtain

$$1-E\left(0;\xi\right)\sim\frac{\beta}{c_0}\left(1-\xi\right)^{2-\left(1+\frac{d'_H}{2}\right)} \tag{231}$$

which gives

$$d_H=1+\frac{d'_H}{2}\ \text{and}\ c_1=\frac{\beta}{c_0}. \tag{232}$$

This result implies that the random walk is a DRWIG. The event of visiting a major site after commencing from some major site is certain to happen, but the mean number of steps to visit is infinite.

As usual, after the parameters d_H and c_1 are determined, we can calculate the effective velocity and the diffusion coefficient from equations (182) and (183),

$$\vartheta=\frac{c_0L\left(\alpha^*-\gamma^*\right)}{\Gamma\left(1+v\left(1-\frac{d'_H}{2}\right)\right)\beta t_0^{v\left(1-\frac{d'_H}{2}\right)}} \tag{233}$$

and

$$D=\frac{c_0\alpha^*L^2}{\Gamma\left(1+v\left(1-\frac{d'_H}{2}\right)\right)\beta t_0^{v\left(1-\frac{d'_H}{2}\right)}}. \tag{234}$$

From these results, the first and the second moments are automatically determined,

$$\langle x\rangle(t)\sim\vartheta t^{v\left(1-\frac{d'_H}{2}\right)} \tag{235}$$

and

$$\left\langle x^2\right\rangle(t)\sim\frac{2\Gamma^2\left(1+v\left(1-\frac{d'_H}{2}\right)\right)}{\Gamma\left(1+2v\left(1-\frac{d'_H}{2}\right)\right)}\langle x\rangle^2(t)+2Dt^{v\left(1-\frac{d'_H}{2}\right)}. \tag{236}$$

As you may notice, the time exponents of the moments are always less than unity even if the PDF of waiting time has the mean, $v=1$. The corresponding transport process is thus in a subdiffusive regime. The qualitative interpretation of this result is that the attachment of major sites with the fractal dangling networks effectively decreases the capability of the random walk to transport along the structure axis.

To find the behavior of the other basic properties, our starting point will be the calculation of equation (186) for branched lattice models,

$$P_{11}(m;\xi)=-\frac{1}{\alpha^*(\xi)}\times\frac{1}{2\pi i}\oint_{\mathcal{C}}\left(z^2-\left(\frac{1}{\alpha^*(\xi)}-\frac{\Sigma(\xi)}{\alpha^*(\xi)}\right)z-\frac{\gamma^*(\xi)}{\alpha^*(\xi)}\right)^{-1}z^{-m}dz \tag{237}$$

where $z\equiv e^{iLk}$ and we have used

$$\left[\text{I-}\overline{\text{p}}(k(z);\xi)\right]^{-1}=\left(1-\left(\gamma^*(\xi)\frac{1}{z}+\Sigma(\xi)+\alpha^*(\xi)z\right)\right)^{-1}. \tag{238}$$

The resulting generating function is (see Appendix 8)

$$P_{11}(m;\xi)=P_{11}^{(1)}(\xi)_{\pm}\times\begin{cases}\left(z_{+}^{(1)}(\xi)\right)^{|m|};m>0\\ \left(z_{-}^{(1)}(\xi)\right)^{|m|};m\le 0\end{cases} \tag{239}$$

where

$$P_{11}^{(1)}(\xi)_{+}=P_{11}^{(1)}(\xi)_{-}=\frac{1}{\sqrt{\left(1-\Sigma(\xi)\right)^2-4\alpha^*(\xi)\gamma^*(\xi)}},$$

$$z_{-}^{(1)}(\xi)=\frac{1}{2\alpha^*(\xi)}\left(\left(1-\Sigma(\xi)\right)-\sqrt{\left(1-\Sigma(\xi)\right)^2-4\alpha^*(\xi)\gamma^*(\xi)}\right),$$

$$z_{+}^{(1)}(\xi)=\frac{1}{2\gamma^*(\xi)}\left(\left(1-\Sigma(\xi)\right)-\sqrt{\left(1-\Sigma(\xi)\right)^2-4\alpha^*(\xi)\gamma^*(\xi)}\right).$$

The result is analogous to that in equation (210). The only difference is the replacement of $\alpha\xi,\gamma\xi,\beta\xi$ by $\alpha^*(\xi),\gamma^*(\xi),\Sigma(\xi)$ respectively.

For the unbiased DRWs, the asymptotic forms of the generating functions $P_{11}^{(1)}(\xi)_{-}$ and $\left(z_{-}^{(1)}(\xi)\right)'$ can be written as

$$P_{11}^{(1)}(\xi)_{-}\sim\frac{1}{2\sqrt{\alpha^*\left(1-E(0;\xi)\right)}}, \tag{240}$$

$$\left(z_{-}^{(1)}(\xi)\right)'\sim-\left(1-E(0;\xi)\right)'P_{11}^{(1)}(\xi)_{-}. \tag{241}$$

Substituting the terms $1-E(0;\xi)$ of equations (223) and (231), which correspond to different kinds of the random walks, into equations (240) and (241), different asymptotic behaviors of the resulting generating functions $P_{11}^{(1)}(\xi)_{-}$ and $\left(z_{-}^{(1)}(\xi)\right)'$, and different values of the parameters c_2 and c_3 are obtained as follows:

For the unbiased DRWFGs,

$$P_{11}^{(1)}(\xi)_{-}\sim\frac{1}{2\sqrt{\alpha^*G}}(1-\xi)^{-\frac{1}{2}}, \tag{242}$$

$$\left(z_{-}^{(1)}(\xi)\right)' \sim \frac{1}{2}\sqrt{\frac{G}{\alpha^*}}(1-\xi)^{-\frac{1}{2}}, \tag{243}$$

$$c_2 = \frac{1}{2\sqrt{\alpha^* G}}, \tag{244}$$

$$c_3 = \frac{1}{2}\sqrt{\frac{G}{\alpha^*}}. \tag{245}$$

For the unbiased DRWIGs,

$$P_{11}^{(1)}(\xi)_{-} \sim \frac{1}{2}\sqrt{\frac{c_0}{\alpha^*\beta}}(1-\xi)^{-\left(1-\frac{1}{2}\left(1+\frac{d_H'}{2}\right)\right)}, \tag{246}$$

$$\left(z_{-}^{(1)}(\xi)\right)' \sim \left(1-\frac{1}{2}\left(1+\frac{d_H'}{2}\right)\right)\sqrt{\frac{\beta}{\alpha^* c_0}}(1-\xi)^{-\frac{1}{2}\left(1+\frac{d_H'}{2}\right)}, \tag{247}$$

$$c_2 = \frac{1}{2}\sqrt{\frac{c_0}{\alpha^*\beta}}, \tag{248}$$

$$c_3 = \left(1-\frac{1}{2}\left(1+\frac{d_H'}{2}\right)\right)\sqrt{\frac{\beta}{\alpha^* c_0}}. \tag{249}$$

As the spectral dimension d_H of the underlying structure is determined by the relation $P_{11}(0;\xi) \sim c_0(1-\xi)^{-(1-d_H/2)}$, from equations (242) and (246), it is clear that the attachment of major sites with finite-size dangling networks does not have an impact on an effective dimensionality to the whole structure but the attachment of major sites with fractal dangling networks does.

It is now a simple matter to calculate the asymptotic values of the probabilities of return to the starting site at large times for the unbiased DRWs. From equation (194) together with equations (224), (232), (244) and (248), the probabilities are therefore, for the unbiased DRWFGs and the unbiased DRWIGs respectively,

$$P_{11}(0,t) \sim \frac{1}{2\Gamma\left(1-\frac{\nu}{2}\right)\sqrt{\alpha^* G}}\left(\frac{t}{t_0}\right)^{-\nu/2}, \tag{250}$$

$$P_{11}(0,t) \sim \frac{1}{2\Gamma\left(1-\frac{\nu}{2}\left(1+\frac{d_H'}{2}\right)\right)}\sqrt{\frac{c_0}{\alpha^*\beta}}\left(\frac{t}{t_0}\right)^{-\frac{\nu}{2}\left(1+\frac{d_H'}{2}\right)}. \tag{251}$$

On the other hand, if the random walk is the biased DRW and the PDF of waiting time shows a power-law tail, $0<\nu<0$, then the limit $P_{11}(0;1^{-})_{-}$ is finite, i.e., $P_{11}(0;1^{-})_{-} = \left|\alpha^* - \gamma^*\right|^{-1}$, and

$$P_{11}(0,t) \sim \frac{1}{\left|\alpha^* - \gamma^*\right| \Gamma(1-\nu)} \left(\frac{t}{t_0}\right)^{-\nu}. \tag{252}$$

According to the inequality of time exponents for these types of random walks, the asymptotic behaviors of the probabilities are in different regimes as illustrated in Figure 21. The unbiased DRWFG is more likely than the unbiased DRWIG to return to the starting site, corresponding to the blue straight line and the green region respectively. It is most unlikely that the biased DRW returns to the starting site, corresponding to the orange straight line.

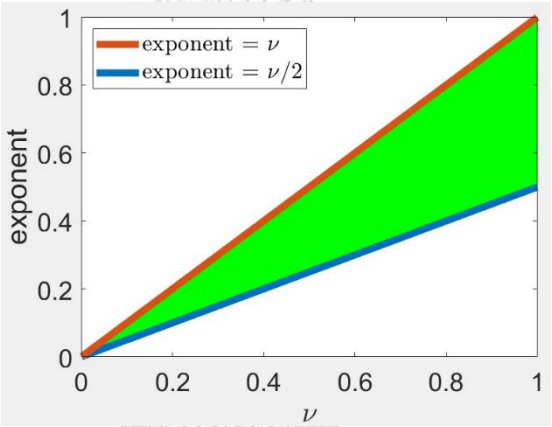


Figure 21. Different regimes of the probability of return to the starting site after long times as characterized by the time exponents.

Even though the diffusions of the unbiased DRWFG and the unbiased DRWIG are in different diffusion regimes, both eventually discover every major site of the underlying structure. The truth is revealed by the probabilities $R_{11}(m)$ of ever reach any major site $\vec{x}_{m,1}$. From the similarity of equations (239) and (210), the probabilities $R_{11}(m)$ are analogous to that in equations (214) – (216) except the single-step transition probabilities α and γ are replaced by the multi-step transition probabilities α^* and γ^* as follows:

$$R_{11}(0) = 1 - \left|\alpha^* - \gamma^*\right|, \tag{253}$$

$$R_{11}(m>0) = \begin{cases} 1 & ;\alpha^* \geq \gamma^* \\ \left(\alpha^*/\gamma^*\right)^{|m|} & ;\alpha^* < \gamma^* \end{cases}, \tag{254}$$

$$R_{11}(m<0)=\begin{cases}\left(\gamma^*/\alpha^*\right)^{|m|} & ;\alpha^*\geq\gamma^* \\ 1 & ;\alpha^*<\gamma^*\end{cases}. \tag{255}$$

As you can see, regardless of types of dangling networks, if the random walk is the unbiased DRW, $\alpha^*=\gamma^*$, then $R_{11}(m)=1$ for every major site. On the other hand, for the biased DRW, $\alpha^*\neq\gamma^*$, if the considered major site is located in the same direction of bias, e.g., $m>0$ and $\alpha^*>\gamma^*$, the event of reaching that site is certain to happen. If the considered major site is located in the opposite direction of bias, e.g., $m<0$ and $\alpha^*>\gamma^*$, the probability of reaching that site decreases exponentially as the distance from the starting site increases.

In spite of certainty of the unbiased DRW reaching every major site, it has been proven that the conditional mean first-passage time to those sites is infinite, i.e., $\tau_{11}(m)=\infty$. This is the reason why the conditional mean first-passage time $\tau_{11}(m,t)$ to a given major site $\vec{x}_{m,1}$ by certain time t has been introduced. It is similar to the other properties. For the DRWFGs and the DRWIGs, $\tau_{11}(m,t)$ behave differently as follows: From equations (195) and (197),

for the unbiased DRWFGs,

$$\tau_{11}(m,t)\sim\frac{vt_0\sqrt{G}}{\Gamma(2-\nu/2)}\left(\frac{t}{t_0}\right)^{1-\nu/2}\times\begin{cases}\sqrt{\alpha^*} & ;m=0\\ |m|/2\sqrt{\alpha^*} & ;m\neq 0\end{cases}. \tag{256}$$

For the unbiased DRWIG,

$$\tau_{11}(m,t)\sim\frac{vt_0\left(1-\left(1+d'_H/2\right)/2\right)}{\Gamma\left(2-\nu\left(1-\left(1+d'_H/2\right)/2\right)\right)}\sqrt{\frac{\beta}{c_0}}\left(\frac{t}{t_0}\right)^{1-\nu\left(1-\left(1+d'_H/2\right)/2\right)}\times\begin{cases}2\sqrt{\alpha^*} & ;m=0\\ |m|/\sqrt{\alpha^*} & ;m\neq 0\end{cases}. \tag{257}$$

It is worth pointing out that the discussion of the conditional mean first-passage times $\tau_{11}(m)$ and $\tau_{11}(m,t)$ can also be applied to the biased DRWFGs when the considered major site $\vec{x}_{m,1}$ is located in the same direction of bias. In this case, the conditional mean first-passage times $\tau_{11}(m)$ and $\tau_{11}(m,t)$ behave differently from that of the unbiased DRWFGs. This can be seen from the finiteness of the mean number of steps to reach the consider major site,

$$\tau_{11}^{(D)}(m\neq 0)=\left|\frac{mG}{\alpha^*-\gamma^*}\right|, \tag{258}$$

which is the essential part of equations (152) and (165) due to $\left(F_{11}\left(m;1^{-}\right)\right)'=\tau_{11}^{(D)}\left(m\right)$. As we have learned, the conditional mean first-passage time $\tau_{11}\left(m\right)$ is the multiplication of the conditional mean number of steps $\tau_{11}^{(D)}\left(m\right)$ and the mean time of the PDF of waiting time. Therefore, for $\nu=1$, it can be shown that

$$\tau_{11}\left(m\neq 0\right)=\left|\frac{mG}{\alpha^{*}-\gamma^{*}}\right|t_0. \tag{259}$$

For $0<\nu<1$, this quantity is divergent, but the conditional mean first-passage time $\tau_{11}\left(m\neq 0,t\right)$ to a given major site $\vec{x}_{m,1}$ by large time t is finite. From equations (165) and (258), we have

$$\tau_{11}\left(m\neq 0,t\right)\sim\left|\frac{mG}{\alpha^{*}-\gamma^{*}}\right|\frac{\nu t_0}{\Gamma\left(2-\nu\right)}\left(\frac{t}{t_0}\right)^{1-\nu}. \tag{260}$$

Finally, from the important parameters we have found and equations (191) and (198), it can be shown that the asymptotic forms of the expected number $\left\langle S\right\rangle\left(t\right)$ of distinct major sites visited after large times are identical to the square roots $\sqrt{\left\langle x^2\right\rangle\left(t\right)}$ except for a rescaling of coefficients, for DRWFGs and DRWIGs respectively,

$$\left\langle S\right\rangle\left(t\right)\sim\begin{cases}\dfrac{2}{\Gamma\left(1+\nu/2\right)}\sqrt{\dfrac{\alpha^{*}}{G}}\left(\dfrac{t}{t_0}\right)^{\frac{\nu}{2}} & ;\vartheta=0\\ \dfrac{\vartheta}{L}t^{\nu} & ;\vartheta\neq 0\end{cases}, \tag{261}$$

$$\left\langle S\right\rangle\left(t\right)\sim\begin{cases}\dfrac{2}{\beta\Gamma\left(1+\nu\left(1-\frac{d_H'}{2}\right)\right)}\sqrt{\dfrac{\alpha^{*}c_0}{\beta}}\left(\dfrac{t}{t_0}\right)^{\frac{\nu}{2}\left(1-\frac{d_H'}{2}\right)} & ;\alpha^{*}=\gamma^{*}\\ \dfrac{c_0\left|\alpha^{*}-\gamma^{*}\right|}{\beta\Gamma\left(1+\nu\left(1-\frac{d_H'}{2}\right)\right)}\left(\dfrac{t}{t_0}\right)^{\nu\left(1-\frac{d_H'}{2}\right)} & ;\alpha^{*}\neq\gamma^{*}\end{cases}, \tag{262}$$

In the previous analysis, we discussed two different kinds of branched lattice models, i.e., the DRWFG and the DRWIG. The goal in this section is to determine the asymptotic behavior of the basic properties of these models. We found that the DRWFG and the DRWIG are in different diffusion regimes. Now it is time to see a demonstration of an application of what we have found. In the following section, we will talk about a comb model and its generalization.

4.3 Sparse comb

As mentioned in the introduction of this thesis, a comb model was proposed as a basic model able to reproduce certain features of transport on fractal medium and percolation clusters. There have been many developments on the problem of random walks on comb-like structures. Previous studies of the comb model have mostly considered the cases that a branch is attached to each site on the backbone (see, e.g., Subsection 1.3.3). Although this model is a simple caricature of various types of natural branched structures, it does not exhaust the whole variety of cases. Therefore, we employ the branched lattice models to study the random walk on modified comb structures, in which attached branches are periodically removed (see

Figure **22**). Here, this kind of structures is called a sparse comb and the sparsity dependence of the random walk properties is of our interest.

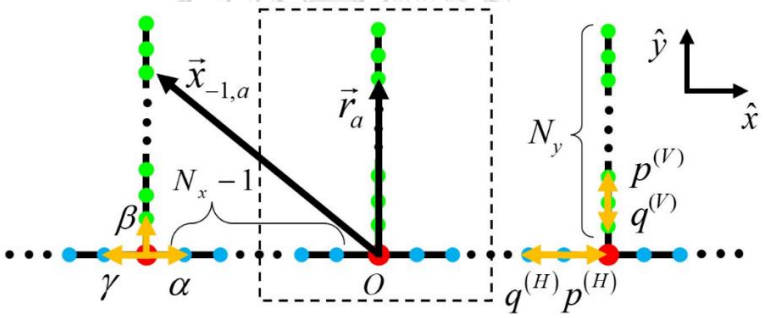


Figure 22. A sparse comb structure with major sites in red spheres, minor sites in blue and green spheres and the orange arrows showing possible single-step transitions of a walker. A dashed line rectangle is illustrated a unit cell.

4.3.1 Model

A sparse comb consists of the backbone connected with branches at major sites. On the backbone, between two nearest major sites, there are $N_x - 1$ minor sites while, on branches, there are N_y minor sites. The unit vector $\hat{x}$ and $\hat{y}$ are set to point along the backbone and the perpendicular direction, respectively. The vectors $N_x\hat{x}$ and $N_y\hat{y}$ define a 2-d rectangle, which is called a unit cell. The unit cell thus contains $N = N_x + N_y$ different sites. The origin O is placed at a certain major site within a unit cell, labelled the 0 th unit cell. Unit cells and sites within each unit

cell are labelled by letters m and a, respectively. The position of the major site within the m th unit cell is thus given by $mN_x\hat{x}$. The relative positions of sites within a unit cell to its major site are denoted by $\vec{r}_1, \vec{r}_2, \vec{r}_3, ..., \vec{r}_N$ where the vector $\vec{r}_1 = 0$ is for the major site itself and the remaining vectors are for minor sites. Accordingly, the position of the a th site in the m th unit cell indicated by the vector $\vec{x}_{m,a}$ may be represented as $\vec{x}_{m,a} = mN_x\hat{x} + \vec{r}_a$ where $a = 1, 2, 3, ..., N$ or the 2-tuple $\left(x_{m,a}, y_{m,a}\right)$. Here, the natural number N_x is regarded as the sparsity of the comb.

The walker walks with nearest neighboring steps with single-step transition probabilities as shown in

Figure **22**. At major sites, the walker may step to the right, the left or the up neighboring sites with probabilities α, γ and β respectively. For walks in branches there is bias towards or away from the backbone depending on whether $p^{(V)}$ is less or more than $1/2$. Similarly, walks on the networks connected two nearest major sites are biased to the left or the right side depending on whether $p^{(H)}$ is less or more than $1/2$.

4.3.2 Results and discussion

From the discussion in Subsection 1.2.8, the n-step transition probabilities $p(1)_n$ and $p(-1)_n$ from a certain major site to the nearest right-hand and left-hand major sites, given that the walker does not visit any major site during the transition, are equal to $\alpha U^{(H)}\left(p^{(H)}, N_x \middle| 1\right)_{n-1}$ and $\gamma U^{(H)}\left(q^{(H)}, N_x \middle| 1\right)_{n-1}$ respectively. Analogously, the n-step transition probability $p(0)_n$ from a certain major site to itself, given that the walker does not visit any major site during the transition, is equal to $\alpha U^{(H)}\left(q^{(H)}, N_x \middle| N_x - 1\right)_{n-1} + \gamma U^{(H)}\left(p^{(H)}, N_x \middle| N_x - 1\right)_{n-1} + \beta U^{(V)}\left(p^{(V)}, N_y\right)_{n-1}$. Hence, we can determine the explicit forms of the transition generating functions as the following equations:

$$\alpha^*(\xi) = \alpha\xi U^{(H)}\left(p^{(H)}, N_x; \xi \middle| 1\right) \tag{263}$$

$$\gamma^*(\xi) = \gamma\xi U^{(H)}\left(q^{(H)}, N_x; \xi \middle| 1\right) \tag{264}$$

$$\begin{aligned}\Sigma(\xi) = \quad & \alpha\xi U^{(H)}\left(q^{(H)}, N_x; \xi \middle| N_x - 1\right) + \gamma\xi U^{(H)}\left(p^{(H)}, N_x; \xi \middle| N_x - 1\right) \\ & + \beta\xi U^{(V)}\left(p^{(V)}, N_y; \xi\right)\end{aligned} \tag{265}$$

where $U^{(H)}\left(p, N; \xi \middle| x_0\right)$ and $U^{(V)}\left(p, N; \xi\right)$ are determined by equations (53) and (59) respectively.

If (i) the length of branches is finite, i.e., $N_y < \infty$, or (ii) the length of branches is infinite and the walker is biased towards to the backbone, i.e., $N_y = \infty$ and $p^{(V)} < 1/2$, then the model is a DRWFG, i.e., $d_H = 1$ and $c_1 = G < \infty$, and the term G can be cast into the following form:

$$G = 1 + \alpha\tau_\alpha\left(p^{(H)}, N_x\right) + \gamma\tau_\gamma\left(p^{(H)}, N_x\right) + \beta\tau_\beta\left(p^{(V)}, N_y\right) \tag{266}$$

where $\tau_\alpha(p, N)$, $\tau_\gamma(p, N)$ and $\tau_\beta(p, N)$ are determined by equations (57), (58) and (60). To determine the parameters c_2 and c_3, we can substitute G and α^* into equations (224), (244) and (245).

It is worth stressing that when $N_y = \infty$, $\lim_{N_y \to \infty} \tau_\beta\left(p^{(V)}, N_y\right)$ is evaluated and in this case $\tau_\beta\left(p^{(V)}, \infty\right) = 1/\left(1 - 2p^{(V)}\right)$. On the other hand, in the limits of $N_y < \infty$ and $p^{(H)} = 0.5$, $G = 1 + (\alpha + \gamma)(N_x - 1) + \beta\tau_\beta\left(p^{(V)}, N_y\right)$, $\tau_\gamma(0.5, N_x) = N_x - 1$ and $\tau_\alpha(0.5, N_x) = N_x - 1$. Furthermore, if the walker is also unbiased in branches, $\lim_{p^{(V)} \to 0.5} \tau_\beta\left(p^{(V)}, N_y\right)$ is evaluated using l'Hospital's rule, and in this case $\tau_\beta(0.5, N_y) = 2N_y - 1$, then $G = 1 + (\alpha + \gamma)(N_x - 1) + \beta(2N_y - 1)$. With that said, when the walker walks symmetrically on a sparse comb with finite-size connected networks, i.e., $\alpha = \gamma = \beta/2 = 1/4$, $p^{(H)} = p^{(V)} = 0.5$ and $1 < N_x, N_y < \infty$, the expected number of steps that the walker walks inside connected networks before returning to a major site is equal to $0.5(N_x + 2N_y)$.

From the previous discussion, it can be shown that if the length of branches is infinite and the walker is unbiased on branches, i.e., $N_y = \infty$ and $p^{(V)} = 0.5$, then the model is a DRWIG. Since the dangling networks are 1-d lattices, the generating function of the corresponding probability of return to the starting site at certain step can be calculated from equation (210) with appropriate parameter associations,

$$P(0; \xi | \beta) = \frac{1}{\xi}\left(1 - \xi^2\right)^{-1/2} \tag{267}$$

which gives

$$c_0 = \frac{1}{\sqrt{2}} \text{ and } d'_H = 1. \tag{268}$$

The straightforward procedure here is to substitute c_0 and d'_H into equation (232), (248) and (249) in order to determine the important parameters. The results are

$$d_H = 3/2,\ c_1 = \beta\sqrt{2}, \tag{269}$$

$$c_2 = \frac{1}{2}\sqrt{\frac{1}{\sqrt{2}\alpha^*\beta}} \text{ and } c_3 = \frac{1}{4}\sqrt{\frac{\sqrt{2}\beta}{\alpha^*}}. \tag{270}$$

Note that the effective dimension of the whole structure is not equal to unity but $3/2$. This leads to the anomalous transport of the DRWIGs.

When the length of branches is infinite and the walker is biased away from the backbone, i.e., $N_y = \infty$ and $p^{(V)} > 0.5$, the model is a NDRW. The probability that the walker leaves a major site and then it is lost in the connected branch does not vanish, i.e.,

$$1 - E_1\left(0;1^-\right) = \beta\left(1 - q^{(V)}/p^{(V)}\right). \tag{271}$$

As mentioned earlier, since after sufficiently long time NDRWs get lost in some branch and the averages of the dynamics properties along the backbone are frozen at certain constants, we will concentrate on DRWs.

We now have all the information at hand to determine the basic random walk properties.

1. The first and the second moments of the walker location along the backbone

For the DRWFGs, the first and the second moments of the random walk along the backbone obey by equations (227) and (228) with $L = N_x$. The effective velocity ϑ and the diffusion coefficient D can be calculated from equations (225) and (226),

$$\vartheta = \frac{\left(\alpha^* - \gamma^*\right)N_x}{\Gamma\left(1+\nu\right)Gt_0^\nu} \tag{272}$$

and

$$D = \frac{\alpha^* N_x^2}{\Gamma\left(1+\nu\right)Gt_0^\nu}. \tag{273}$$

We find that if the transition probability $p^{(H)}$ is equal to the first magic number defined by

$$p_1^{(H)} \equiv \left(1+\left(\gamma/\alpha\right)^{1/(1-N_x)}\right)^{-1}, \tag{274}$$

then the effective velocity vanishes (see Appendix 9). In the case that $\alpha=\gamma$, $p_1^{(H)}$ is equal to 0.5, and it does not depend on the sparsity N_x. Hence, to simplify the discussion, for this subsection, when the term "unbiased random walk" is used here, it will be understood that we refer specifically that $\alpha=\gamma$ and $p^{(H)}=0.5$. This also implies that $\alpha^*=\gamma^*=\alpha/N_x$.

It can be shown that if the transition probability $p^{(H)}$ is identical to the second magic number defined by

$$p_2^{(H)} \equiv \frac{1}{2}\left(1+\frac{\alpha-\gamma}{1+\beta\tau_\beta}\right), \tag{275}$$

the effective velocity does not vanish, and it does not depend on the sparsity (see Appendix 10), i.e., $\vartheta=\left(\alpha-\gamma\right)\Big/\left(\left(1+\beta\tau_\beta\right)\Gamma\left(1+\nu\right)t_0^\nu\right)$. Furthermore, for $\alpha>\gamma$, if $p^{(H)}>p_2^{(H)}$, the motion along the backbone is enhanced by increasing the sparsity while if $0.5<p^{(H)}<p_2^{(H)}$, the motion is diminished. Figure 23 (left) demonstrates these results. It is similar for $\alpha<\gamma$. If $p^{(H)}<p_2^{(H)}$, the motion along the backbone is enhanced by increasing the sparsity while if $0.5>p^{(H)}>p_2^{(H)}$, the motion is diminished.

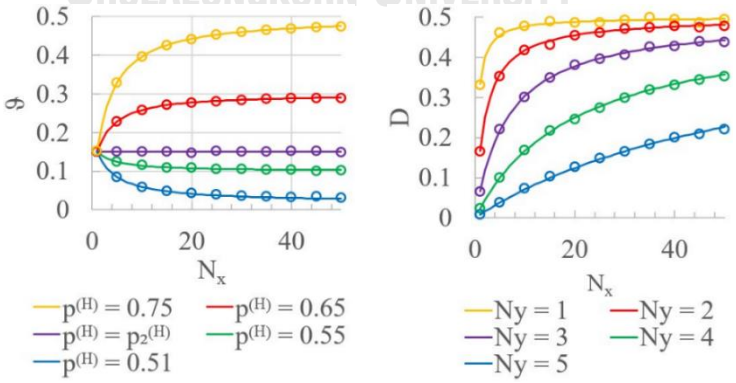


Figure 23. The sparsity dependence of the effective velocity (left) and the diffusion coefficient (right). Solid curves correspond to exact analytical results. Results from numerical simulations are depicted with circles.

Asymptotically, when the sparsity is increased, the effective velocity and the diffusion coefficient of the random walks biased and unbiased along the backbone saturate at $\frac{p^{(H)}-q^{(H)}}{\Gamma(1+\nu)t_0^{\nu}}$ and $\frac{1}{2\Gamma(1+\nu)t_0^{\nu}}$ respectively. For $\nu=1$, these are the values corresponding to a perfect 1-d lattice model with associating appropriate parameters (see equations (204) and (205)). These are illustrated in Figure 23 where we have used $\alpha=0.4$, $\gamma=0.1$, $p^{(V)}=0.25$, $N_y=5$, $\nu=1$ and $t_0=1$ (left), and $\alpha=\gamma=0.4$, $p^{(V)}=0.5$, $\nu=1$ and $t_0=1$ (right).

As we said, when $p^{(V)}=0.5$ and $N_y=\infty$, the random walk is a DRWIG. From equations (233) - (236) with the result (269), we find that, for large time t,

$$\langle x\rangle(t)\sim\frac{N_x\left(\alpha^*-\gamma^*\right)}{\beta\sqrt{2}\Gamma(1+\nu/2)}\left(\frac{t}{t_0}\right)^{\nu/2} \tag{276}$$

and

$$\left\langle x^2\right\rangle\sim\frac{2\Gamma^2(1+\nu/2)}{\Gamma(1+\nu)}\langle x\rangle^2(t)+\frac{\sqrt{2}N_x\alpha}{\beta\Gamma(1+\nu/2)}\left(\frac{t}{t_0}\right)^{\nu/2}. \tag{277}$$

It should be remarked that the exponent is halved comparing with the one of the DRWFGs. This is because, for the DRWIGs, the existence of connected branches "strongly" affects the dynamics of random walks along the backbone. Although the transport process is "slower" than usual, the one of the DRWFGs, the walker is still able to diffuse along the backbone. The second moment along the backbone corresponds to subdiffusion when the walker is unbiased along the backbone. Interestingly, in the limit of the biased random walk, the prefactor of the second moment is the function of square of the sparsity for large sparsity while, in the limit of the unbiased random walk, the prefactor is proportional to the sparsity instead.

For the NDRWs, $p^{(V)}>0.5$ and $N_y=\infty$, from equations (111), (112) and (271), we find that the first and the second moments can be estimated from the following equations:

$$\langle x\rangle(t)\sim\frac{N_x\left(\alpha^*-\gamma^*\right)}{\beta\left(\left|p^{(V)}-q^{(V)}\right|/p^{(V)}\right)} \tag{278}$$

and

$$\left\langle x^2 \right\rangle(t) \sim \frac{N_x^2\left(\alpha^* + \gamma^*\right)}{\beta\left(\left|p^{(V)} - q^{(V)}\right| / p^{(V)}\right)} + 2\left(\frac{N_x\left(\alpha^* - \gamma^*\right)}{\beta\left(\left|p^{(V)} - q^{(V)}\right| / p^{(V)}\right)}\right)^2. \tag{279}$$

As you can see, there is no time t appearing on the righthand side of the equations. This can be interpreted that at large times the walker is lost in some branches and stochastic localization occurs [62].

In Figure 24, we compare the analytical results of the first and the second moments with numerical simulations for the random walks on sparse combs with infinite length branches, $N_y = \infty$. As you can see, they display the three different transport behaviors depending on the degrees of bias on branches $p^{(V)}$.

When the sparsity is unity or $N_x = 1$, the corresponding model is a simple comb model. If the random walk is unbiased along the backbone, i.e., $\alpha = \gamma = 1/4$ and $\beta = 1/2$, we find that our analytical results are in agreement with the results found in [34], which are derived by the different formalism, i.e., the generalized master equation combined with the method of Kahng and Redner [63].

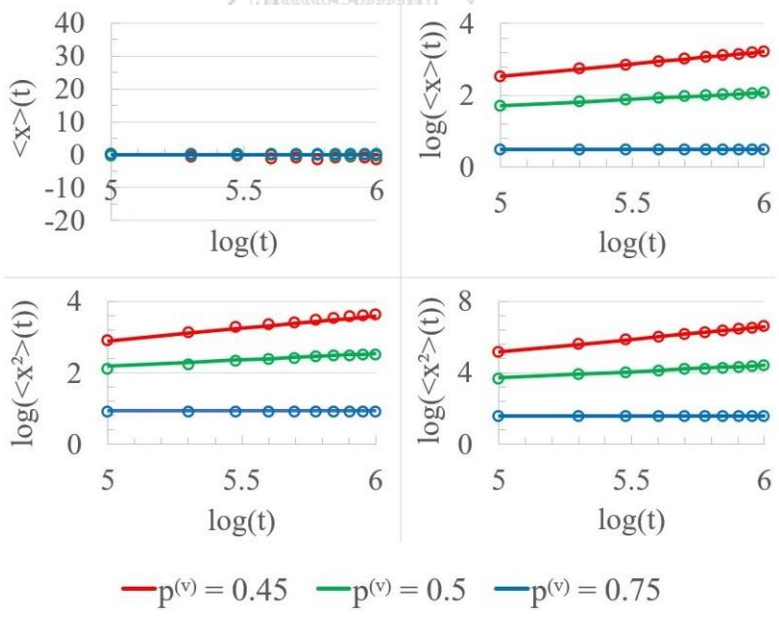


Figure 24. The first and the second moments of random walks unbiased (left) with $\alpha = \gamma = 1/4$ and $p^{(H)} = 0.5$, and biased (right) with $\alpha = 0.3$, $\gamma = 0.1$, $p^{(H)} = 0.75$ on the backbone with $N_x = 5$ and $N_y = \infty$ for three different values of $p^{(V)} = 0.25, 0.5, 0.75$. The exponent v of the PDF of waiting time is equal to 0.7.

2. The probability of return to the starting site

For the case that the value of $\left(P_{11}\left(0;1^{-}\right)\right)^{-1}$ is not zero, e.g., biased DRWs and NDRWs, the probability $P_{11}\left(0,t\right)$ of return to the starting site after large time t can be described by equation (141). The value of $\left(P_{11}\left(0;1^{-}\right)\right)^{-1}$ can be calculated from equation (239), respectively,

$$\left(P_{11}\left(0;1^{-}\right)\right)^{-1}=\left|\alpha^{*}-\gamma^{*}\right|, \tag{280}$$

$$\left(P_{11}\left(0;1^{-}\right)\right)^{-1}=\sqrt{\left(\alpha^{*}+\gamma^{*}+\beta\left(1-\frac{q^{(v)}}{p^{(v)}}\right)\right)^{2}-4\alpha^{*}\gamma^{*}}\,. \tag{281}$$

For unbiased DRWFGs, the asymptotic behavior of $P_{11}\left(0,t\right)$ obeys equation (250). In the limit of large sparsity, its prefactor approaches the one for a perfect 1-d lattice, i.e., $\frac{t_0^{v/2}}{2\sqrt{2}\alpha\Gamma\left(1-v/2\right)}$, when $v=1$. On the other hand, for unbiased DRWIGs, from the result (268) together with equation (251), it leads to

$$P_{11}\left(0,t\right)\sim\frac{1}{\Gamma\left(1-3v/4\right)}\sqrt{\frac{N_x}{4\sqrt{2}\alpha\beta}}\left(\frac{t}{t_0}\right)^{-3/4}. \tag{282}$$

For large sparsity, this result is in contrast with the result of the DRWFGs because the prefactor in equation (282) does not saturate at any constant, but it is proportional to the square root of the sparsity.

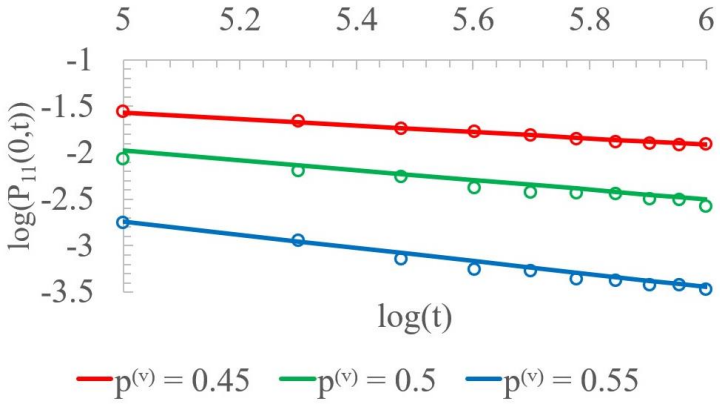


Figure 25. The graphs of the asymptotic behaviors of the probability of return to the starting site at large time t. Lines correspond to results given by equations (250),

(251) and (141) for $p^{(V)}=0.45$ (red), $p^{(V)}=0.5$ (green) and $p^{(V)}=0.55$ (blue) respectively. Symbols correspond to results from numerical simulations.

The verification of the analytical results is confirmed by the numerical results shown in Figure 25. The numerical results were obtained by using $\alpha=\gamma=0.1$, $p^{(H)}=0.5$, $N_x=5$, $N_y=\infty$ and $v=0.7$. According to the infinity of length of branches, the probability of return to the starting site also displays the three different behaviors depending on the value of $p^{(V)}$.

3. The probability of ever reaching a given major site

For DRWs, as we have known, the probability of ever reaching the starting site obeys equation (253). For other major sites, the probabilities of ever reaching those sites obey equations (254) and (255). In sparse comb models, we find that if the transition probability $p^{(H)}$ is equal to the third magic number defined by

$$p_3^{(H)} \equiv \frac{1}{1+\gamma/\alpha}, \tag{283}$$

then the sparsity has no impact on the probability of ever reaching the starting site. This is because the term $\alpha^*-\gamma^*$ is independent of the sparsity (see Appendix 11), i.e., $\alpha^*-\gamma^*=\alpha-\gamma$. It is analogous to the effective velocity ϑ. For $\alpha>\gamma$, if $p^{(H)}>p_3^{(H)}$, the walk moving away from the starting site along the backbone is enhanced by increasing the sparsity while if $0.5<p^{(H)}<p_3^{(H)}$, the walk is diminished. It is similar for $\alpha<\gamma$. We need just switch the inequality signs. Figure 26 demonstrates these results.

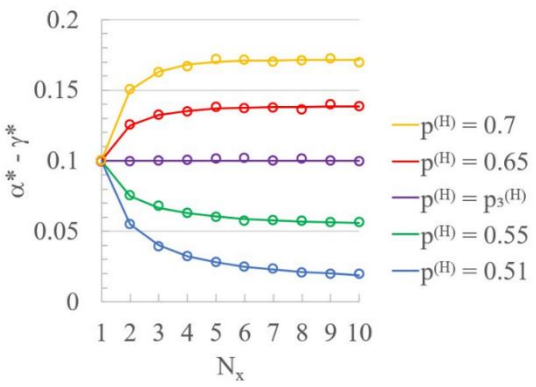


Figure 26. The sparsity dependence of $\alpha^* - \gamma^*$ with using $\alpha = 0.3$, $\gamma = 0.3$, $p^{(V)} = 0.25$ and $N_y = 5$. The numerical results (circles) fit by using equations (263) and (264).

In addition, the below equation shows the asymptotic values of $\alpha^* - \gamma^*$ as $N_x \to \infty$ for $p^{(H)} \neq p_3^{(H)}$,

$$\alpha^* - \gamma^* \sim \begin{cases} \alpha\left(p^{(H)} - q^{(H)}\right)\Big/ p^{(H)} & p^{(H)} > 0.5 \\ \left(\alpha - \gamma\right)/N_x & p^{(H)} = 0.5 \\ \gamma\left(p^{(H)} - q^{(H)}\right)\Big/ q^{(H)} & p^{(H)} < 0.5 \end{cases} . \quad (284)$$

4. The conditional mean first-passage time to a given major site

For given the PDF of waiting time with finite mean time, $\nu = 1$, the conditional mean first-passage time $\tau_{11}(m)$ to a given major site $\vec{x}_{m,1}$ is determined by the conditional mean number $\tau_{11}^{(D)}(m) \equiv \left(F_{11}(m;1)\right)' \Big/ R_{11}(m)$ of steps that the walker takes before visiting that site for the first time. For the sparse comb models, since the explicit forms of the transition generating functions are shown in equations (263) through (265), $\tau_{11}^{(D)}(m)$ can be calculated by using equations (92), (239), (253) – (255). In general, the resulting expression is nontrivial. However, for biased DRWFGs, to calculate $\tau_{11}(m)$ which $\vec{x}_{m,1}$ is located in the same direction of bias, we only need to calculate G and $\left|\alpha^* - \gamma^*\right|$, and plug them into equation (259).

As we have learned, in the case of the unbiased DRWFGs, the conditional mean first-passage time to a certain major site is infinite but the event that the walker eventually reaches that major site is certain. Thus, for unbiased DRWFGs, we can calculate the conditional mean first passage time $\tau_{11}(m,t)$ to a given major site by large time t from equation (256).

For unbiased DRWIGs, the asymptotic forms of $\tau_{11}(m,t)$ can be expressed by using equation (257) together with (268),

$$\tau_{11}(m,t) \sim \frac{vt_0}{\Gamma(2-v/4)}\sqrt{\frac{\beta}{2\sqrt{2}}}\left(\frac{t}{t_0}\right)^{1-v/4} \times \begin{cases} \sqrt{\frac{\alpha}{N_x}} & m=0 \\ \frac{|m|}{2}\sqrt{\frac{N_x}{\alpha}} & m\neq 0 \end{cases} . \quad (285)$$

It is remarkable that the coefficients of $\tau_{11}(0,t)$ and $\tau_{11}(m\neq 0,t)$ depend inversely on the square root of the sparsity.

5. The expected number of distinct major sites visited

For DRWFGs, the expected number $\langle S\rangle(t)$ of distinct major sites visited after long time t can be calculated by equation (261) with $L=N_x$. The effective velocity ϑ, the limit α^* and the mean steps G can be calculated by using equations (263) through (265). For large sparsity, $v=1$ and associating appropriate parameters, the prefactors of the result are identical to those for a perfect 1-d lattice except for the division by the sparsity N_x,

$$\langle S\rangle(t) \sim \begin{cases} \frac{\sqrt{2}}{N_x\Gamma(1+v/2)}\left(\frac{t}{t_0}\right)^{v/2} & ;\vartheta=0 \\ \frac{p^{(H)}-q^{(H)}}{N_x\Gamma(1+v)}\left(\frac{t}{t_0}\right)^{v} & ;\vartheta\neq 0 \end{cases} . \quad (286)$$

For the DRWIGs, we can express the asymptotic form of $\langle S\rangle(t)$ by using equations (262) and (268),

$$\langle S\rangle(t) \sim \begin{cases} \frac{1}{\Gamma(1+v/4)}\sqrt{\frac{2\sqrt{2}\alpha}{\beta N_x}}\left(\frac{t}{t_0}\right)^{v/4} & ;|\alpha^*-\gamma^*|=0 \\ \frac{|\alpha^*-\gamma^*|}{\beta\sqrt{2}\Gamma(1+v/2)}\left(\frac{t}{t_0}\right)^{v/2} & ;|\alpha^*-\gamma^*|\neq 0 \end{cases} . \quad (287)$$

On one hand, for $|\alpha^*-\gamma^*|=0$ and large sparsity, its coefficient is inversely proportional to the square root of the sparsity. On the other hand, for $|\alpha^*-\gamma^*|=0$ and large sparsity, its coefficient may be independent of or inversely proportional to the sparsity (see equation (284)).

For NDRWs, if equations (271) and (281) are plugged into equation (174), after rearranging terms, we will find that $\langle S\rangle(t)$ can be estimated as

$$\langle S\rangle(t)\sim\frac{p^{(V)}\sqrt{\left(\alpha^*+\gamma^*+\beta\left(1-q(V)/p^{(V)}\right)\right)^2-4\alpha^*\gamma^*}}{\beta\left|p^{(V)}-q^{(V)}\right|} \tag{288}$$

which is independent of time t. This is consistent with the asymptotic behavior of the first and the second moments, the walker does not diffuse along the backbone and discover any new major sites at long times.

6. Discussion

We were able to show the closed-form expression of the generating function $P_{11}(m;\xi)$ of the probability $P_{11}(m)_n$ that the walker is found at a given major site $\vec{x}_{m,1}$ at the nth step. For the random walker walking symmetrically on non-sparse combs with infinite-length branches, i.e., $N_x=1$ and $N_y=\infty$, our result is identical to the 2-d comb result of P. Illien and O. B´enichou (see Eq. (31) in [7]).

For the random walk on sparse combs, we found that if the transition probability $p^{(H)}$ is equal to $p_1^{(H)}\equiv\left(1+(\gamma/\alpha)^{1/(1-N_x)}\right)^{-1}$, the random walk is unbiased along the backbone, i.e., $\mathcal{G}=0$. In the limit of $\alpha=\gamma$, $p_1^{(H)}$ is equal to 0.5 independent of the sparsity N_x. Therefore, to simplify the discussion, in this subsection, the term "unbiased random walk" is meant that $\alpha=\gamma$ and $p^{(H)}=0.5$.

For the unbiased DRWFGs, we found that the considered properties depend on the sparsity N_x monotonically. For the biased DRWFGs, the monotonicity is determined by the effective velocity $\mathcal{G}=\frac{\left(\alpha^*-\gamma^*\right)N_x}{\Gamma(1+\nu)Gt_0^{\nu}}$ (and the degrees of bias $\alpha^*-\gamma^*$). We found that if the $\mathcal{G}$ ($\alpha^*-\gamma^*$) does not depend on the sparsity, i.e., $\mathcal{G}=(\alpha-\gamma)\Big/\left((1+\beta\tau_\beta)\Gamma(1+\nu)t_0^{\nu}\right)$ ($\alpha^*-\gamma^*=\alpha-\gamma$), then the term $p^{(H)}$ is identical to $p_2^{(H)}\equiv\frac{1}{2}\left(1+\frac{\alpha-\gamma}{1+\beta\tau_\beta}\right)$ ($p_3^{(H)}\equiv\frac{1}{1+\gamma/\alpha}$). Furthermore, for $\alpha>\gamma$, if $p^{(H)}>p_2^{(H)}$ ($p_3^{(H)}$), the value of $|\mathcal{G}|$ ($\left|\alpha^*-\gamma^*\right|$) is monotonically increased as the sparsity is increased while if $0.5<p^{(H)}<p_2^{(H)}$ ($p_3^{(H)}$), the value is monotonically decrease as the sparsity is increased. It is similar for $\alpha<\gamma$. We need just switch the inequality signs. Figure 27 demonstrates the example surfaces of $p_1^{(H)}$, $p_2^{(H)}$ and $p_3^{(H)}$ in green,

red and blue respectively, by using $N_x = 5$ and $\tau_\beta = 5$. For the DRWFGs with $\nu = 1$, in the limit of large sparsity, the random walk properties are independent of the sparsity and identical to those for a 1-d lattice.

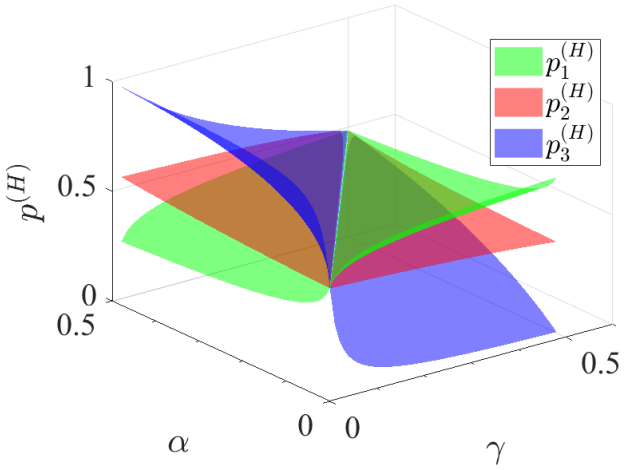


Figure 27. The surfaces of three magic numbers $p_1^{(H)}$, $p_2^{(H)}$ and $p_3^{(H)}$.

For the DRWIGs, the existence of branches "strongly" affects the dynamics of random walks along the backbone. Although the transport process is "slower" than usual, the one of the DRWFGs, the walker is still able to diffuse along the backbone. This can be deduced from the changes of the exponents of the basic statistical properties comparing with those for the DRWFGs. For instance, for the second moment of the unbiased random walk, the exponent is halved, i.e., $\langle x^2 \rangle(t) \sim \frac{\sqrt{2} N_x \alpha}{\beta \Gamma(1+\nu/2)} \left(\frac{t}{t_0} \right)^{\nu/2}$ which corresponds to the well-known result of subdiffusive transport. In the case of the DRWIGs, the considered properties still monotonically depend on the sparsity, but the results are not identical to those for a perfect 1-d lattice as the sparsity is large. For the unbiased random walk on a non-sparse comb, i.e., $N_x = 1$, our analytical results of the second moment are in agreement with the results found in [34], which are derived by the different formalism, i.e., the generalized master equation combined with the method of Kahng and Redner [63].

For the NDRWs, the length of branches is infinite, and the walker is biased outward from the backbone. After long times the walker is lost in some branches and the averages of the dynamics properties along the backbone are frozen.

4.4 Conclusion and discussion

In this chapter, we employed the GFF to obtain the asymptotic behavior of basic statistical properties of the separable continuous-time random walks on branched lattices, consisting of periodically repeated unit cells with the following properties: in the unit cell, (i) there exists one major site, which is connected to its equivalent sites in neighboring unit cells by a certain kind of network; and (ii) there may be a dangling network attached to the major site. The crux of the formalism for this model is to focus attention on the generating functions $\alpha^*(\xi)$, $\gamma^*(\xi)$ and $\Sigma(\xi)$ of the multi-step transition probabilities that the walker leaves a major site and enters connected networks before arriving at the right, the left nearest major sites and the commencing major site, respectively, without visiting other major sites.

The main results are as the follows. For the branched lattices with finite-size networks connected to major sites and the PDF of waiting time possessing the mean, we find that the asymptotic forms of the basic random walk properties are identical to those for a perfect 1-d lattice except for a rescaling of coefficients. On the other hand, for the branched lattices with fractal dangling networks attached to major sites, if the spectral dimension d'_H of the attached fractals is in the interval $(0,2)$, then the spectral dimension of the whole structure will be $d_H = 1 + \frac{d'_H}{2}$. Furthermore, the capability of the random walk to transport along the structure axis decreases as the spectral dimension of the attached fractals increases.

If the unit cell of a branched structure contains a major site, which is connected to its equivalent sites by a 1-d lattice with finite length N_x, and a dangling 1-d lattice is attached to the major site. Here, the structure is named the sparse comb and the length N_x is regarded as the sparsity of the structure. The steps along the branches and the structure axis may be biased. It was shown that if the length of branches is infinite, then the transport process displays the three

different behaviors depending on the bias probability $p^{(V)}$ on branches. Moreover, it was also demonstrated that a simple relation appears between an exponent $0<\nu\leq 1$ characterizing the asymptotic behavior of the Laplace transform of the PDF of waiting time, $\psi^*(s)\sim 1-(t_0 s)^{\nu}$, and the basic statistical properties.

We also found that the effective velocity ϑ and the degree of bias $\left|\alpha^*-\gamma^*\right|$ along the backbone depend on the sparsity N_x monotonically. In the situations that these quantities vanish, the corresponding model is called the random walk "unbiased" along the backbone. It was found that when the random walk is unbiased, it does not have to walk symmetrically, i.e., $\alpha\neq\gamma$ and $p^{(H)}\neq 0.5$ where $p^{(H)}$ is defined as the transition probability to the neighboring right site in a finite 1-d lattice connected two nearest major sites, α and γ are defined respectively as the transition probabilities from a major site to the right and the left neighboring sites.

This fact led us to the interesting findings. For given $\alpha\neq\gamma$, there exists a magic number $p_1^{(H)}\neq 0.5$ such that if $p^{(H)}=p_1^{(H)}$ then the random walk is unbiased. On the other hand, for the biased diffusive random walk with the finite mean number of steps returning to major sites, it could be shown that if $p^{(H)}$ is equal to one of the two magic numbers, called $p_2^{(H)}$ and $p_3^{(H)}$, which are also the functions of the transition probabilities, then certain random walk properties are independent of the sparsity N_x. The diagram in Fig. 10 demonstrates the surfaces corresponding to the magic numbers.

The concrete models have been so far analyzed based on the assumption that, in each unit cell, there is only one major site. Therefore, the rest of this work is devoted to generalizing the analysis to other solvable multi major-site models, i.e., ladder models and cylindrical models respectively.

5

Random walks on ladder lattices

This chapter is about a random walk description of the non-deterministic transport of a particle on ladder-like structures. A ladder structure we propose here is a quasi-1d infinite structure, consisting of two parallel rails (1-d infinite lattices) periodically connected to each other with rungs (1-d finite lattices). The walker steps along these different components of the ladder may be biased differently. We employ the GFF to analyze the basic statistical properties of this random walk model. As compared with the DRWFGs on branched lattices, we find that although the additional structure does not affect the exponents, it does have a great impact on the prefactors.

5.1 Model

Unlike the previously considered structures, a "ladder" is a quasi-1d infinite structure whose each unit cell contains two different major sites as shown in Figure 28. In this chapter, for convenience, let us distinguish these two major sites by the plus-minus sign instead of the numbers. In each unit cell, the $+$ major site is connected to the $-$ major site with a N_y-length 1-d lattice, called a "rung", and the $\pm$ major site is connected to its nearest $\pm$ major sites in the next unit cell with a N_x-length 1-d lattice. There are thus $N = N_x + N_y + 2$ different sites in each unit cell. The lines passing through all $\pm$ major sites are called the "$\pm$ rail". For sake of simplicity, the distance between neighboring sites is set to be unity.

We employ here the same coordinate system of the previous chapters. The origin O is placed at a certain major site on the $+$ rail within a unit cell, labelled the 0th unit cell. Unit cells and sites within each unit cell are labelled by letters m and a, respectively. The position of the $+$ major site within the mth unit cell is thus

given by $m\left(N_x+1\right)\hat{x}$. The relative positions of sites within a unit cell to the $+$ major site are denoted by $\vec{r}_+,\vec{r}_-,\vec{r}_1,\vec{r}_2,\vec{r}_3,...,\vec{r}_{N_x+N_y}$ where the vectors $\vec{r}_+=0$ and $\vec{r}_-=\left(N_y+1\right)\hat{y}$ are respectively for the major site itself and the other major site, and the remaining vectors are for minor sites. Accordingly, the position of the a th site in the m th unit cell indicated by the vector $\vec{x}_{m,a}$ may be represented as $\vec{x}_{m,a}=m\left(N_x+1\right)\hat{x}+\vec{r}_a$ where $a=\pm,1,2,3,...,N_x+N_y$ or $\left(x_{m,a},y_{m,a}\right)$.

A walker located at the $+$ major site may jump to the right, left, or up neighboring sites with probabilities α_+, γ_+ and $\beta_+=1-\alpha_+-\gamma_+$ respectively. Similarly, the walker located at the $-$ major site may jump to the right, left, or down neighboring sites with probabilities α_-, γ_- and $\beta_-=1-\alpha_--\gamma_-$ respectively. However, when the walker is at a minor site on rungs, it can jump to the up or down neighboring sites with probabilities $p^{(V)}$ and $q^{(V)}=1-p^{(V)}$ respectively. If the walker is at the minor site on the $\pm$ rail, it may jump to the right and left neighboring sites with probabilities $p_\pm^{(H)}$ and $q_\pm^{(H)}=1-p_\pm^{(H)}$ respectively. In addition, between successive steps, the walker waits for a random time t distributed according to a general probability distribution function $\psi\left(t\right)$ whose the Laplace transform is asymptotically $\psi^*\left(s\right)\sim1-\left(t_0s\right)^\nu$ where $t_0>0$ and $0<\nu\leq1$.

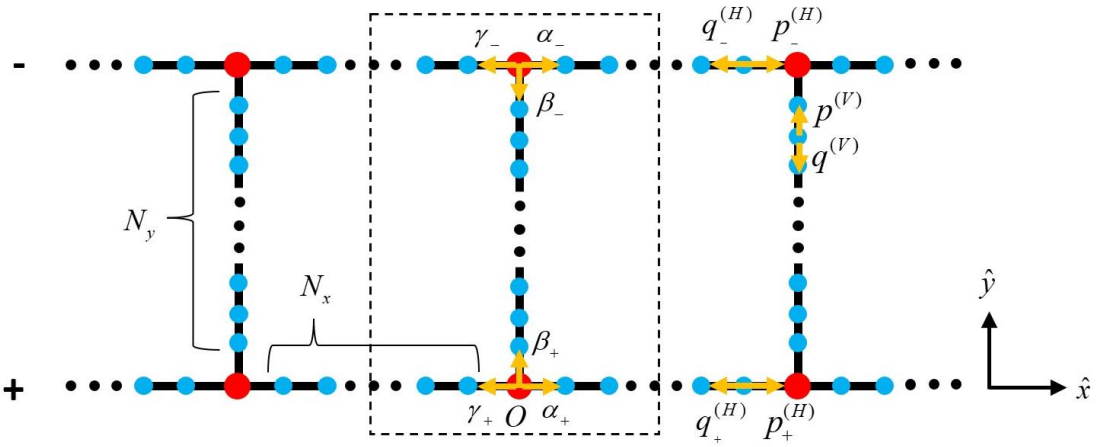


Figure 28. A ladder structure with major sites (red spheres), minor sites (blue spheres) and the orange arrows showing possible transitions.

5.2 General cases

Before turning to our specific cases of ladder models, we set down in the present section certain relationship of general validity for systems of this type. Let us first consider the matrix $\bar{\mathrm{p}}(k;\xi)$. Since the connected network between two nearest major sites is a finite 1-d lattice, it is not difficult to adopt the results of Subsection 1.2.8 to the generating functions $p_{ab}(\Delta m;\xi)$ of the n-step transition probabilities $p_{ab}(\Delta m)_n$ from a major site $\vec{x}_{0,b}$ to a major site $\vec{x}_{\Delta m,a}$. For convenience of further analysis, let us define certain functions as the follows: For $a,b=\pm$ and $\Delta m=-1,0,1$,

$$\lambda_{ab}(\Delta m;\xi)_{\pm}\equiv\frac{1\pm\sqrt{1-4\rho_{ab}(\Delta m)\left(1-\rho_{ab}(\Delta m)\right)\xi^2}}{2\xi\rho_{ab}(\Delta m)}$$

where $\rho_{ab}(\Delta m)\equiv\begin{cases}p_a^{(H)} & ,\Delta m=1,a=b\\ 1-p_a^{(H)} & ,\Delta m=-1,a=b\\ p^{(V)} & ,\Delta m=0,a=-,b=+\\ 1-p^{(V)} & ,\Delta m=0,a=+,b=-\end{cases}$,

$$\chi_{ab}(\Delta m)\equiv\begin{cases}\alpha_a & ,\Delta m=1,a=b\\ \gamma_a & ,\Delta m=-1,a=b\\ \beta_b & ,\Delta m=0,a=-b\end{cases}\text{ and }N_{ab}\equiv\begin{cases}N_x+1 & ,a=b\\ N_y+1 & ,a=-b\end{cases}.$$

From these definitions, if the destination major site and the commencing major site are different, i.e., $(\Delta m,a,b)\in\{(-1,\pm,\pm),(1,\pm,\pm),(0,\mp,\pm)\}$, we have

$$p_{ab}(\Delta m;\xi)=\xi\chi_{ab}(\Delta m)\left(\frac{\lambda_{ab}(\Delta m;\xi)_+-\lambda_{ab}(\Delta m;\xi)_-}{\lambda_{ab}^{N_{ab}}(\Delta m;\xi)_+-\lambda_{ab}^{N_{ab}}(\Delta m;\xi)_-}\right). \tag{289}$$

Vice versa, if the destination major site and the commencing major site are the same, i.e., $(\Delta m,a,b)\in\{(0,\pm,\pm)\}$, we have

$$\begin{aligned}p_{bb}(0;\xi)= \quad & \xi\chi_{bb}(1)\left(\frac{\lambda_{bb}^{N_x}(-1;\xi)_+-\lambda_{bb}^{N_x}(-1;\xi)_-}{\lambda_{bb}^{N_x+1}(-1;\xi)_+-\lambda_{bb}^{N_x+1}(-1;\xi)_-}\right)+\\ & \xi\chi_{bb}(-1)\left(\frac{\lambda_{bb}^{N_x}(1;\xi)_+-\lambda_{bb}^{N_x}(1;\xi)_-}{\lambda_{bb}^{N_x+1}(1;\xi)_+-\lambda_{bb}^{N_x+1}(1;\xi)_-}\right)+\\ & \xi\chi_{-bb}(0)\left(\frac{\lambda_{-bb}^{N_y}(0;\xi)_+-\lambda_{-bb}^{N_y}(0;\xi)_-}{\lambda_{-bb}^{N_y+1}(0;\xi)_+-\lambda_{-bb}^{N_y+1}(0;\xi)_-}\right)\end{aligned}. \tag{290}$$

Afterwards, the matrix $\bar{\mathrm{p}}(k;\xi)$ can be expressed as

$$\bar{\mathrm{p}}(k;\xi)=\begin{bmatrix}\bar{p}_{++}(k;\xi) & \bar{p}_{+-}(k;\xi)\\ \bar{p}_{-+}(k;\xi) & \bar{p}_{--}(k;\xi)\end{bmatrix} \tag{291}$$

where

$$\bar{p}_{++}(k;\xi) \equiv e^{-i(N_x+1)k}\gamma_+^*(\xi) + \Sigma_+(\xi) + e^{i(N_x+1)k}\alpha_+^*(\xi),$$
$$\bar{p}_{--}(k;\xi) \equiv e^{-i(N_x+1)k}\gamma_-^*(\xi) + \Sigma_-(\xi) + e^{i(N_x+1)k}\alpha_-^*(\xi),$$
$$\bar{p}_{+-}(k;\xi) \equiv \beta_-^*(\xi) \text{ and } \bar{p}_{-+}(k;\xi) \equiv \beta_+^*(\xi).$$

To unclutter the notation, we have used $\alpha_\pm^*(\xi)$, $\gamma_\pm^*(\xi)$, $\beta_\pm^*(\xi)$ and $\Sigma_\pm(\xi)$ as short-hand notations for $p_{\pm\pm}(1;\xi)$, $p_{\pm\pm}(-1;\xi)$, $p_{\mp\pm}(0;\xi)$ and $p_{\pm\pm}(0;\xi)$ respectively.

From fundamentals of linear algebra, the eigenfunctions $E_\pm(k;\xi)$ and the eigenvector $\pi(k;\xi)$ of the matrix $\bar{\mathrm{p}}(k;\xi)$ can be found from

$$E_\pm(k;\xi) = \frac{1}{2}\left(\mathrm{Tr}\left[\bar{\mathrm{p}}(k;\xi)\right] \pm \sqrt{\left(\mathrm{Tr}\left[\bar{\mathrm{p}}(k;\xi)\right]\right)^2 - 4\det\left[\bar{\mathrm{p}}(k;\xi)\right]}\right) \tag{292}$$

where $\mathrm{Tr}\left[\bar{\mathrm{p}}(k;\xi)\right]$ is the sum of elements on the diagonal of the matrix $\bar{\mathrm{p}}(k;\xi)$,

$$\pi(k;\xi) = \frac{1}{\bar{p}_{+-}(k;\xi) + \bar{p}_{-+}(k;\xi)}\begin{bmatrix} \bar{p}_{+-}(k;\xi) \\ E_+(k;\xi) - \bar{p}_{++}(k;\xi) \end{bmatrix}. \tag{293}$$

It is worth stressing that, after taking limit, we obtain $E_+(0;1^-) = 1$ and

$$\begin{bmatrix} \pi_+ \\ \pi_- \end{bmatrix} = \frac{1}{\beta_+^* + \beta_-^*}\begin{bmatrix} \beta_-^* \\ \beta_+^* \end{bmatrix}. \tag{294}$$

This equation implies that, regardless of minor sites, the probability $\pi_\pm$ of finding the walker at the $\pm$ major site at large times equals to the multi-step transition probability $\beta_\mp^*$ from the $\mp$ major site to the $\pm$ major site divided by $\beta_+^* + \beta_-^*$.

From the finiteness of the size of the connected networks, it can be shown that the random walker is a DRWFG,

$$1 - E_-(0;\xi) \sim (1-\xi)G, \tag{295}$$

which gives

$$c_1 = G \text{ and } d_H = 1, \tag{296}$$

where

$$G = \begin{array}{l} \left(\alpha_+\tau_\alpha\left(p_+^{(H)}, N_x+1\right) + \gamma_+\tau_\gamma\left(p_+^{(H)}, N_x+1\right) + \beta_+\tau_\alpha\left(p^{(V)}, N_y+1\right)\right)\pi_+ + \\ \left(\alpha_-\tau_\alpha\left(p_-^{(H)}, N_x+1\right) + \gamma_-\tau_\gamma\left(p_-^{(H)}, N_x+1\right) + \beta_-\tau_\gamma\left(p^{(V)}, N_y+1\right)\right)\pi_- + 1 \end{array}. \tag{297}$$

As you can see, the spectral dimension of ladders is unity. Therefore, for the random walk on ladders, if the PDF of waiting time possessing the mean, the normal transport should be expected.

Let us now calculate the effective velocity $\mathcal{G}$ and the diffusion coefficient D by substituting the entries $\overline{p}_{ab}\left(k;1^{-}\right)$ into equations (182) and (183). We find that

$$\mathcal{G}=\frac{\left(N_x+1\right)\left\langle \alpha^{*}-\gamma^{*}\right\rangle}{\Gamma\left(1+\nu\right)Gt_0^{\nu}} \tag{298}$$

and

$$D=\frac{\left(N_x+1\right)^2\left\langle \alpha^{*}\right\rangle}{\Gamma\left(1+\nu\right)Gt_0^{\nu}} \tag{299}$$

where, for any variable $\sigma_{\pm}$ associating with the $\pm$ rail, $\langle\sigma\rangle\equiv\pi_{-}\sigma_{-}+\pi_{+}\sigma_{+}$ is denoted as the weighted average of that variable.

To a certain extent, the finding results of random walks on ladders may be used to investigate transport properties of models with media possessing two diffusivities. Therefore, the contribution of these diffusivities to the effective diffusivity should be of interest. Figure 29 illustrates the contribution of the single-step transition probabilities on the $+$ rail and the $-$ rail to the quantities relevant to the diffusive properties of the random walk, i.e., $\left\langle \alpha^{*}-\gamma^{*}\right\rangle$, G, $\mathcal{G}$ and D.

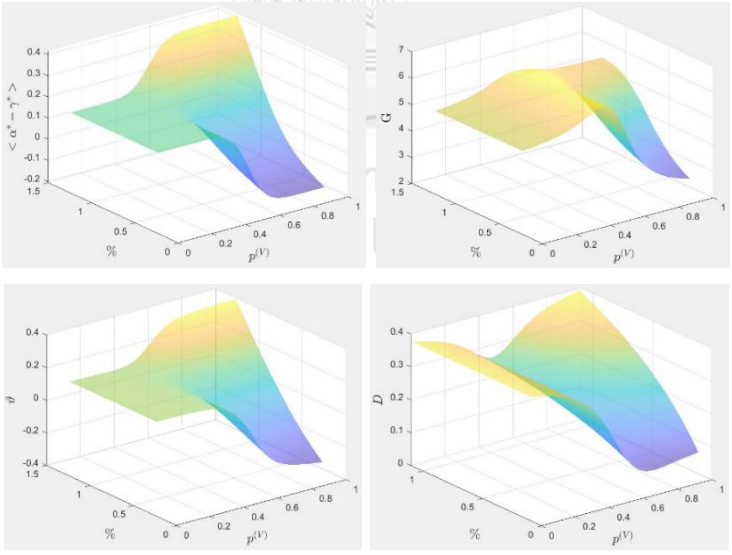


Figure 29. The surfaces of four quantities $\left\langle \alpha^{*}-\gamma^{*}\right\rangle$, G, $\mathcal{G}$ *and* D for the case that $\nu=1$, $t_0=1$ and $N_x=N_y=5$. With the single-step transition probabilities on the $+$ rail fixed, i.e., $\alpha_{+}=0.5$, $p_{+}^{(H)}=0.6$, the probabilities on the $-$ rail, i.e., $\alpha_{-}\equiv\%\alpha_{+}$, $p_{-}^{(H)}\equiv\%\,p_{+}^{(H)}$, and $p^{(V)}$, are varied where $\%$ and $p^{(V)}$ are in the intervals $\left(0.25,1.25\right)$ and $\left(0,1\right)$ respectively.

As you can see, when the value of $p^{(V)}$ is intermediate, the single-step transition probabilities on both rails have an impact on these four quantities. On the other hand, if the value of $p^{(V)}$ is close to 0 or 1, the localized transition on the corresponding rail dominates the four quantities.

After determining the important parameters, i.e., d_H, ϑ and D, we have the following relations, which permit us to calculate the first and the second moments of the walker location along the rails at large times;

$$\langle x \rangle(t) \sim \vartheta t^{\nu} \tag{300}$$

and

$$\langle x^2 \rangle(t) \sim \frac{2\Gamma^2(1+\nu)}{\Gamma(1+2\nu)} \langle x \rangle^2(t) + 2Dt^{\nu}. \tag{301}$$

To verify our analytical results, the numerical simulations of the unbiased random walks on the ladder are performed by varying values of the diffusion coefficient and the characteristic exponent of the PDF of waiting time, i.e., $\nu = 0.7, 0.75, 0.8$. The numerical results are shown in Figure 30. They are plotted by varying t with abscissa $\log(t)$ and ordinate $\log\left(\langle x^2 \rangle(t)/2D\right)$. As expected, the analytical results have good agreements with the numerical results, the plots of the same value of ν fall on the same curve.

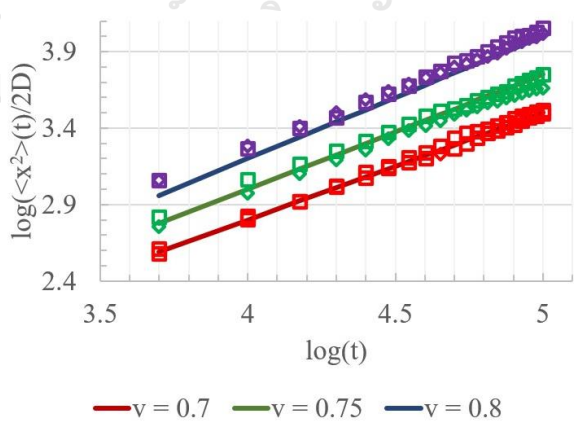


Figure 30. The scaling numerical results of the second moments of the unbiased random walks, which are represented with symbols. Solid curves correspond to exact analytical results.

In view of the GFF, to obtain the other basic properties, the explicit form of the generating function $P_{ab}(m;\xi)$ is desired. However, the problem of finding $P_{ab}(m;\xi)$ by equation (186) with the matrix $\bar{\mathrm{p}}(k;\xi)$ determined by equation (291) is relevant to solving a quartic equation which is very complicated. More precisely, we need to find the roots z of the equation $\det\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(k(z);\xi\right)\right]=0$ or

$$\left(1-\bar{p}_{++}\left(k(z);\xi\right)\right)\left(1-\bar{p}_{--}\left(k(z);\xi\right)\right)-\bar{p}_{-+}\left(k(z);\xi\right)\bar{p}_{+-}\left(k(z);\xi\right)=0 \tag{302}$$

where $z\equiv e^{i(N_x+1)k}$.

Accordingly, we may make progress to the extent that we can overcome this complication. What follows, we will consider two special cases which the quartic equation problem is reduced to the quadratic equation. As we will show next, in both cases, the resulting generating functions $P_{ab}(m;\xi)$ can be expressed in the form

$$P_{ab}(m;\xi)=\left(z_{\pm}^{(1)}(\xi)\right)^{|m|}P_{ab}^{(1)}(\xi)_{\pm}+\left(z_{\pm}^{(2)}(\xi)\right)^{|m|}P_{ab}^{(2)}(\xi)_{\pm}. \tag{303}$$

5.3 Horizontally symmetrical random walks

First, we consider the horizontally symmetrical random walks, in the sense that the single-transition probabilities are satisfied the following conditions:

$$\alpha\equiv\alpha_{+}=\alpha_{-},\ \gamma\equiv\gamma_{+}=\gamma_{-},\ p^{(H)}\equiv p_{+}^{(H)}=p_{-}^{(H)}\ \text{and}\ p^{(V)}=\frac{1}{2}. \tag{304}$$

This implies that $\gamma^{*}(\xi)\equiv\gamma_{+}^{*}(\xi)=\gamma_{-}^{*}(\xi)$, $\alpha^{*}(\xi)\equiv\alpha_{+}^{*}(\xi)=\alpha_{-}^{*}(\xi)$, $\beta^{*}(\xi)\equiv\beta_{+}^{*}(\xi)=\beta_{-}^{*}(\xi)$, $\Sigma(\xi)\equiv\Sigma_{+}(\xi)=\Sigma_{-}(\xi)$ which yield

$$\bar{p}_{++}(k;\xi)=\bar{p}_{--}(k;\xi)=e^{-i(N_x+1)k}\gamma^{*}(\xi)+\Sigma(\xi)+e^{i(N_x+1)k}\alpha^{*}(\xi),$$
$$\bar{p}_{-+}(k;\xi)=\bar{p}_{+-}(k;\xi)=\beta^{*}(\xi).$$

In words, the transitions on both rails are identical. From this identity, for convenience, let us hereafter omit the plus-minus sign for the single-step transition probabilities and the corresponding generating functions.

As a result of the restriction in equation (304), equation (302) becomes

$$\left(1-\left(z^{-1}\gamma^{*}(\xi)+\Sigma(\xi)+z\alpha^{*}(\xi)\right)\right)^{2}-\left(\beta^{*}(\xi)\right)^{2}=0 \tag{305}$$

and the inverse $\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(k(z);\xi\right)\right]^{-1}$ can be written as

$$\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(k(z);\xi\right)\right]^{-1}=\frac{\begin{bmatrix}\bar{p}_{++}\left(k(z);\xi\right) & -\bar{p}_{-+}\left(k(z);\xi\right)\\ -\bar{p}_{-+}\left(k(z);\xi\right) & \bar{p}_{++}\left(k(z);\xi\right)\end{bmatrix}}{\left(1-\left(z^{-1}\gamma^{*}(\xi)+\Sigma(\xi)+z\alpha^{*}(\xi)\right)\right)^{2}-\left(\beta^{*}(\xi)\right)^{2}}. \tag{306}$$

By substituting this inverse into equation (186) and using the residue theorem (see Appendix 12), we arrive at the result

$$P_{ab}(m;\xi)=\left(z_{\pm}^{(1)}(\xi)\right)^{|m|}P_{ab}^{(1)}(\xi)+\left(z_{\pm}^{(2)}(\xi)\right)^{|m|}P_{ab}^{(2)}(\xi) \tag{307}$$

where

$$z_{-}^{(1)}(\xi)=\frac{\Phi_{-}(\xi)-\Gamma_{-}(\xi)}{2\alpha^{*}(\xi)}, \tag{308}$$

$$z_{-}^{(2)}(\xi)=\frac{\Phi_{+}(\xi)-\Gamma_{+}(\xi)}{2\alpha^{*}(\xi)} \tag{309}$$

with $z_{+}^{(1)}(\xi)=\frac{\alpha^{*}(\xi)}{\gamma^{*}(\xi)}z_{-}^{(1)}(\xi)$, $z_{+}^{(2)}(\xi)=\frac{\alpha^{*}(\xi)}{\gamma^{*}(\xi)}z_{-}^{(2)}(\xi)$, $\Phi_{\pm}(\xi)\equiv 1-\Sigma(\xi)\pm\beta^{*}(\xi)$ and $\Gamma_{\pm}(\xi)\equiv\sqrt{\Phi_{\pm}^{2}(\xi)-4\gamma^{*}(\xi)\alpha^{*}(\xi)}$, and

$$P_{++}^{(1)}(\xi)=\frac{1}{2\Gamma_{-}(\xi)}, \tag{310}$$

$$P_{++}^{(2)}(\xi)=\frac{1}{2\Gamma_{+}(\xi)} \tag{311}$$

with $P_{++}^{(1)}(\xi)=P_{+-}^{(1)}(\xi)=P_{--}^{(1)}(\xi)=P_{-+}^{(1)}(\xi)$ and $P_{-+}^{(2)}(\xi)=P_{+-}^{(2)}(\xi)=-P_{--}^{(2)}(\xi)=-P_{++}^{(2)}(\xi)$. For the convenience of calculation, let us show the limit values of certain generating functions as the follows; $\Phi_{+}=\gamma^{*}+\alpha^{*}+2\beta^{*}$, $\Phi_{-}=\gamma^{*}+\alpha^{*}$, $\Gamma_{-}=\left|\gamma^{*}-\alpha^{*}\right|$ and $\Gamma_{+}=\sqrt{\left(\gamma^{*}-\alpha^{*}\right)^{2}+\beta^{*}\left(2\left(\gamma^{*}+\alpha^{*}\right)+\beta^{*}\right)}$.

We now have all the information at hand to determine the remaining basic properties of the random walk. However, before moving on, let us emphasize here that, for the rest of this section, we will concentrate solely on the biased random walk because the unbiased random walk is the special case of the other case which we will discuss in the next section.

As the first basic property of the random walk for a given major site, we consider the probability $P_{bb}(0,t)$ of return to the starting site $\vec{x}_{0,b}$. Its asymptotic form can be determined by substituting the limit $P_{bb}(0;1^{-})$ of equation (307) into equation (188), for $0<\nu<1$,

$$P_{bb}(0,t)\sim\frac{1}{\Gamma(1-\nu)\left(1-R_{bb}(0)\right)}\left(\frac{t}{t_{0}}\right)^{-\nu} \tag{312}$$

where $R_{bb}(0)=1-1/P_{bb}(0;1^{-})$ or

$$R_{bb}(0)=1-2\frac{\Gamma_{-}\Gamma_{+}}{\Gamma_{-}+\Gamma_{+}}. \tag{313}$$

Recall that $R_{bb}(0)$ is the probability of ever return to the starting major site. For the biased random walk which implies $|\alpha^{*}-\gamma^{*}|\neq 0$, it can be shown that $R_{bb}(0)$ cannot equal to unity. Moreover, as the degree of bias $|\alpha^{*}-\gamma^{*}|$ increases, the event of ever return to the starting major site is less likely to happen, in which the value of the prefactor of $P_{bb}(0,t)$ also decreases.

Unlike an unrestricted 1-d lattice and branched lattices, ladders possess two primary axes, i.e., the + and the − rails. Therefore, although the considered major site is located in the same direction of bias, e.g., $m>0$ and $\alpha^{*}-\gamma^{*}>0$, intuitively the event of reaching that major site is not certain. This statement can be proved by considering the probability of ever reach $R_{ab}(m)$ for $m\neq 0$. According to equations (189) and (307), we have

$$R_{ab}(m)=\frac{\Gamma_{+}}{\Gamma_{+}+\Gamma_{-}}\left(z_{\pm}^{(1)}\right)^{|m|}\pm\frac{\Gamma_{-}}{\Gamma_{+}+\Gamma_{-}}\left(z_{\pm}^{(2)}\right)^{|m|} \tag{314}$$

where the use of color has been employed to reduce confusion for the reader. The red plus (minus) sign is selected when $a=b$ ($a\neq b$), and the blue plus (minus) sign is selected when $m>0$ ($m<0$). This worth pointing out that, from equations (308) and (309), for $\alpha^{*}-\gamma^{*}>0$, if $m>0$, then $z_{+}^{(1)}=1$ and $z_{+}^{(2)}<1$, while, if $m<0$, then $z_{-}^{(1)},z_{-}^{(2)}<1$. Clearly, the analogous statement can also be made about $\alpha^{*}-\gamma^{*}<0$. Consequently, for the case that the considered major site is located in the same direction of bias, equation (314) becomes

$$R_{ab}(m)=\frac{\Gamma_{+}}{\Gamma_{+}+\Gamma_{-}}\pm\frac{\Gamma_{-}}{\Gamma_{+}+\Gamma_{-}}\left(z_{\pm}^{(2)}\right)^{|m|} \tag{315}$$

which is always less than unity. Asymptotically, for $|m|\gg 0$, this equation reduces to

$$R_{ab}(m)\approx\frac{\Gamma_{+}}{\Gamma_{+}+\Gamma_{-}}. \tag{316}$$

In addition, for the case that the considered major site is located in the opposite direction of bias, it can be shown that

$$R_{ab}(m)\approx 0. \tag{317}$$

The following figures illustrate the changes of the probabilities $R_{++}(m)$ under different conditions. The left figure shows the $p^{(H)}$ and N_x dependence of the probability $R_{++}(0)$ of eventually return to the starting site. Interestingly, at the short length N_x, the value of $p^{(H)}$ contributed to the peak of $R_{++}(0)$ is not equal to 0.5. However, when the length N_x is increased, the value of $p^{(H)}$ approaches 0.5.

The right figure illustrates the accuracy of the analytical results and the approximations. The blue and the red solid curves correspond to the analytical results for $R_{++}(m)$ and $R_{-+}(m)$ respectively, and the green solid curve corresponds to the approximations. Results from numerical simulations are depicted with circles.

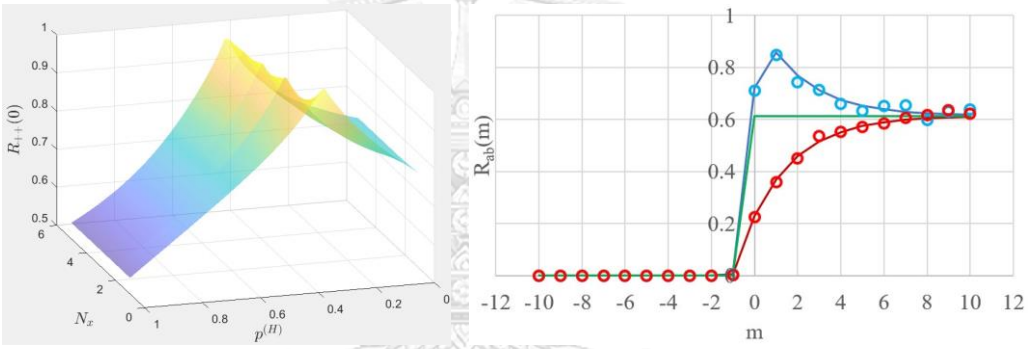


Figure 31. Illustrations of the changes of the probabilities $R_{ab}(m)$ under different conditions. For both figures, the condition that $\alpha = 0.4$, $\gamma = 0.2$, $N_y = 5$, $\nu = 1$ and $t_0 = 1$ was used. For the left figure, the values of N_x and $p^{(H)}$ are varied in the intervals $[1,5]$ and $(0,1)$ respectively. For the right figure, these values are fixed, i.e., $N_x = 5$ and $p^{(H)} = 0.7$.

For the cases that the PDF of waiting time possessing the mean, i.e., $\nu = 1$, to make the description of the event of reach a given major more complete, the conditional mean first-passage time $\tau_{ab}(m)$ to that site should be taken into account. The explicit form of $\tau_{ab}(m)$ can be obtained by substituting equation (307) into equation (190) followed with lengthy rearrangement,

$$\frac{\tau_{bb}(0)}{t_0} = \frac{\left(1 - R_{++}(0)\right)^2}{2R_{++}(0)} \left(\frac{|\Gamma'_-|}{\Gamma_-^2} + \frac{|\Gamma'_+|}{\Gamma_+^2} \right) \tag{318}$$

and

$$\frac{\tau_{ab}(m\neq 0)}{t_0}=\frac{1-R_{aa}(0)}{R_{ab}(m)}\left(P_{ab}(m)\right)'-\frac{R_{aa}(0)}{1-R_{aa}(0)}\tau_{ab}(0) \tag{319}$$

where

$$\begin{aligned}\left(P_{ab}(m)\right)' = & \frac{\left(z_{\pm}^{(1)}\right)^{|m|}}{2\Gamma_{-}}\left(|m|\left(\frac{\Phi'_{-}-\Gamma'_{-}}{\Phi_{-}-\Gamma_{-}}-\frac{\left(C^{*}\right)'}{C^{*}}\right)+\frac{|\Gamma'_{-}|}{\Gamma_{-}}\right) \\ & \pm\frac{\left(z_{\pm}^{(1)}\right)^{|m|}}{2\Gamma_{-}}\left(|m|\left(\frac{\Phi'_{-}-\Gamma'_{-}}{\Phi_{-}-\Gamma_{-}}-\frac{\left(C^{*}\right)'}{C^{*}}\right)+\frac{|\Gamma'_{-}|}{\Gamma_{-}}\right)\end{aligned} \tag{320}$$

with $C^{*}(m;\xi)\equiv\begin{cases}\alpha^{*}(\xi) & ;m>0\\ \gamma^{*}(\xi) & ;m<0\end{cases}$.

The complex form of $\tau_{ab}(m\neq 0)$ in equation (319) is reduced to a more compact form when the considered major site is in the same direction of bias and far from the starting site, i.e., $|m|\gg 0$,

$$\tau_{ab}(m)\approx|m|\left(\frac{\Phi'_{-}-\Gamma'_{-}}{\Phi_{-}-\Gamma_{-}}-\frac{\left(C^{*}\right)'}{C^{*}}\right)t_0. \tag{321}$$

As you can see, although the conditional mean time is proportional to the "distance" from the starting major site to the considered major site, it is not in the form of the distance divided by the absolute value of the effective velocity, like the previous models.

Let us end this section by considering the expected number $\langle S\rangle(t)$ of distinct major sites visited. Aside from the previous basic properties for a given major site, the expected number $\langle S\rangle(t)$ is also governed by the probability $R_{++}(0)$ of ever return to the starting site. This can be seen from the asymptotic form of $\langle S\rangle(t)$ which can be obtained from equation (191) with $N_M=2$, $\pi_{\pm}=1/2$, $c_1=G$, $d_H=1$, and $1/P_{++}(0;1^{-})=1-R_{++}(0)$,

$$\langle S\rangle(t)\sim\frac{1-R_{++}(0)}{G\Gamma(1+\nu)}\left(\frac{t}{t_0}\right)^{\nu}. \tag{322}$$

Figure 32 shows that the analytical results have a good agreement with the numerical results. The numerical simulations are performed for different conditions and the characteristic exponent of the PDF of waiting time, i.e., $\nu=0.7,0.75,0.8$. The

numerical results, which are represented by symbols, are plotted by varying t with abscissa $\log(t)$ and ordinate $\log\left(\frac{\langle S\rangle(t)}{S_0}\right)$ where $S_0 \equiv \frac{1-R_{++}(0)}{G\Gamma(1+\nu)t_0^{\nu}}$. Clearly, the plots of the same value of ν fall on the same curve.

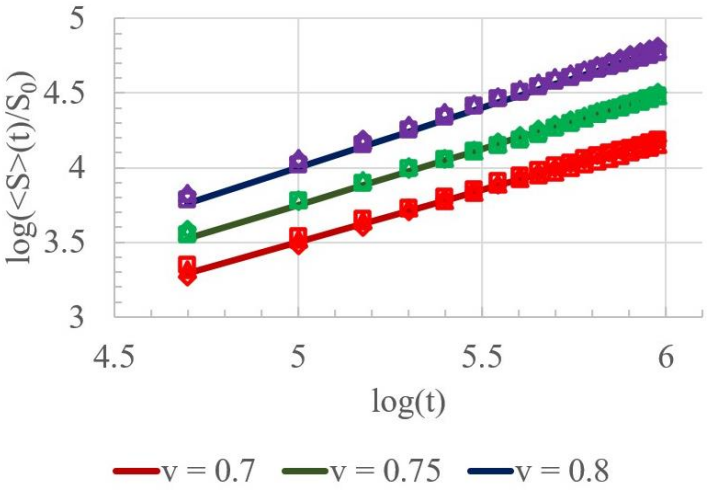


Figure 32. The scaling numerical results of the expected number $\langle S\rangle(t)$, which are represented with symbols. Solid curves correspond to exact analytical results.

5.4 Vertically symmetrical random walks

In this section we discuss the second special case of the ladder models, the vertically symmetrical random walk, in the sense that the single-transition probabilities are satisfied the following conditions:

$$\alpha_{\pm} = \gamma_{\pm} \text{ and } p_{\pm}^{(H)} = \frac{1}{2}. \tag{323}$$

This implies that $\gamma_{\pm}^{*}(\xi) = \alpha_{\pm}^{*}(\xi)$ which yields

$$\bar{p}_{\pm\pm}(k;\xi) = \left(e^{-i(N_x+1)k} + e^{i(N_x+1)k}\right)\alpha_{\pm}^{*}(\xi) + \Sigma_{\pm}(\xi),$$

$$\bar{p}_{\mp\pm}(k;\xi) = \beta_{\pm}^{*}(\xi).$$

In words, the events that the walker takes a jump to the left and the right neighboring site always have the identical transition probabilities. This also tells us that the effective velocity always vanishes, which means that the random walk is an unbiased random walk along the structure axis.

As a result of the restriction in equation (323), equation (302) becomes

$$\prod_{a=\pm}\left(1-\left(\alpha_a^*(\xi)\left(z+z^{-1}\right)+\Sigma_a(\xi)\right)\right)-\prod_{a=\pm}\beta_a^*(\xi)=0 \tag{324}$$

and the inverse $\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(k(z);\xi\right)\right]^{-1}$ can be written as

$$\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(k(z);\xi\right)\right]^{-1}=\frac{\begin{bmatrix}\bar{p}_{--}\left(k(z);\xi\right) & -\bar{p}_{+-}\left(k(z);\xi\right)\\ -\bar{p}_{-+}\left(k(z);\xi\right) & \bar{p}_{++}\left(k(z);\xi\right)\end{bmatrix}}{\prod_{a=\pm}\left(1-\left(\alpha_a^*(\xi)\left(z+z^{-1}\right)+\Sigma_a(\xi)\right)\right)-\prod_{a=\pm}\beta_a^*(\xi)}. \tag{325}$$

Note that, to shorten some equations in the following paragraph, we will omit the arguments of functions appeared in the right side of the equations. In addition, in accordance with the symmetry of the model which yields $z_+^{(1,2)}(\xi)=z_-^{(1,2)}(\xi)$ and $P_{ab}^{(1,2)}(\xi)_+=P_{ab}^{(1,2)}(\xi)_-$, we will omit the plus-minus-sign subscripts of these terms.

By substituting this inverse into equation (186) and using the residue theorem (see Appendix 12 and 13), we arrive at the result

$$P_{ab}(m;\xi)=\left(z^{(1)}(\xi)\right)^{|m|}P_{ab}^{(1)}(\xi)+\left(z^{(2)}(\xi)\right)^{|m|}P_{ab}^{(2)}(\xi). \tag{326}$$

where

$$z^{(1,2)}(\xi)=B_{1,2}(\xi)-\sqrt{B_{1,2}^2(\xi)-1}, \tag{327}$$

for $B_{1,2}(\xi)\equiv\frac{\alpha_-^*\left(1-\Sigma_+\right)+\alpha_+^*\left(1-\Sigma_-\right)\pm K}{4\alpha_+^*\alpha_-^*}$, the minus sign is for $B_1(\xi)$ and the plus sign is for $B_2(\xi)$, and

$$K(\xi)\equiv\sqrt{\left(2\alpha_-^*\left(1-\Sigma_+\right)+2\alpha_+^*\left(1-\Sigma_-\right)\right)^2-16\alpha_+^*\alpha_-^*\left(\left(1-\Sigma_+\right)\left(1-\Sigma_-\right)-\beta_-^*\beta_+^*\right)}.$$

The remaining terms in equation (326) are

$$P_{++}^{(1)}(\xi)=-\frac{\left(2B_1-D_1\right)\alpha_-^*}{K\sqrt{B_1^2-1}},\ P_{--}^{(1)}(\xi)=-\frac{\left(2B_1-D_2\right)\alpha_+^*}{K\sqrt{B_1^2-1}}, \tag{328}$$

for $D_1(\xi)\equiv\frac{1}{\alpha_-^*(\xi)}\left(1-\Sigma_-(\xi)\right)$ and $D_2(\xi)\equiv\frac{1}{\alpha_+^*(\xi)}\left(1-\Sigma_+(\xi)\right)$, and

$$P_{+-}^{(1)}(\xi)=\frac{\beta_-^*}{K\sqrt{B_1^2-1}},\ P_{-+}^{(1)}(\xi)=\frac{\beta_+^*}{K\sqrt{B_1^2-1}},\ P_{++}^{(2)}(\xi)=\frac{\left(2B_2-D_1\right)\alpha_-^*}{K\sqrt{B_2^2-1}},$$

$$P_{--}^{(2)}(\xi)=\frac{\left(2B_2-D_2\right)\alpha_+^*}{K\sqrt{B_2^2-1}},\ P_{+-}^{(2)}(\xi)=-\frac{\beta_-^*}{K\sqrt{B_2^2-1}}\ \text{and}\ P_{-+}^{(2)}(\xi)=-\frac{\beta_+^*}{K\sqrt{B_2^2-1}}.$$

The asymptotic forms of the terms $P_{bb}^{(1)}(\xi)$ and $\left(z^{(1)}(\xi)\right)'$ can be obtained from formulas (327) and (328), $P_{bb}^{(1)}(\xi)\sim\frac{\pi_b\left(1-\xi\right)^{-1/2}}{2\sqrt{\langle\alpha^*\rangle G}}$ and $\left(z^{(1)}(\xi)\right)'\sim\frac{1}{2}\sqrt{\frac{G}{\langle\alpha^*\rangle}}\left(1-\xi\right)^{-1/2}$

which lead to

$$c_2 = \frac{1}{2\sqrt{\langle \alpha^* \rangle G}} \tag{329}$$

and

$$c_3 = \frac{1}{2}\sqrt{\frac{G}{\langle \alpha^* \rangle}}\,. \tag{330}$$

We can calculate the asymptotic behavior of all the basic properties of the random walk from these relations together with results (296).

The probability of return to the starting site at large time t is

$$P_{bb}(0,t) \sim \frac{\pi_b}{2\Gamma\left(1-\frac{\nu}{2}\right)\sqrt{\langle \alpha^* \rangle G}}\left(\frac{t}{t_0}\right)^{-\nu/2} \tag{331}$$

for $0 < \nu \leq 1$. The resemble between this result and the result (250) for the unbiased DRWFGs on branched lattices should be noted. However, we find that because of the existence of two major sites in each unit cell which leads to the occurrence of the term $\pi_b < 1$. This means that the unbiased random walk on the ladder L is less likely than the unbiased DRWFG on the branched lattice B to return to the starting site if the both models have the same values of the means of steps taking inside connected networks, i.e., $G_L = G_B$, and the multi-step transition probabilities, i.e., $\langle \alpha_L^* \rangle = \alpha_B^*$.

As we have learned for the unbiased random walks on quasi-1d infinite structures, consideration for the probability $R_{ab}(m)$ of ever reaching a given major site and the conditional mean first-passage time $\tau_{ab}(m)$ leads us to the paradox that the walker is certain to be at every site on the structure, i.e., $R_{ab}(m) = 1$, but we must wait for long time generally, i.e., $\tau_{ab}(m) = \infty$. This is one of the reasons why the more informative quantity, the conditional mean first-passage time $\tau_{ab}(m,t)$ to a given major site by a certain time t, is introduced. The important parameters, e.g., c_2 and c_3, have already been determined so, from equations (195) through (197), what we obtain are as follows; For the starting major site,

$$\tau_{\pm\pm}(0,t) \sim \frac{\nu t_0}{\Gamma(2-\nu/2)\pi_\pm}\sqrt{G\langle \alpha^* \rangle}\left(\frac{t}{t_0}\right)^{1-\nu/2}, \tag{332}$$

for the other major sites in the starting unit cell,

$$\tau_{\pm\mp}(0,t) \sim \left(P_{\pm\pm}^{(2)} - P_{\pm\mp}^{(2)}\right)\tau_{\pm\pm}(0,t) \tag{333}$$

and, for the remaining major sites,

$$\tau_{ab}(m,t) \sim \frac{vt_0|m|}{2\Gamma(2-v/2)}\sqrt{\frac{G}{\langle\alpha^*\rangle}}\left(\frac{t}{t_0}\right)^{1-v/2}. \tag{334}$$

It was noticed that on one hand, for $m \neq 0$, the conditional mean first-passage time $\tau_{ab}(m,t)_L$ of the unbiased random walk on the ladder L is equal to the conditional mean first-passage time $\tau_{ab}(m,t)_B$ of the unbiased DRWFG on the branched lattice B in equation (256) if both models have the same values of the means of steps taking inside connected networks and the multi-step transition probabilities. On the other hand, for $m=0$, the $\tau_{bb}(0,t)_L$ is not equal to $\tau_{bb}(0,t)_B$ but it is $1/\pi_b$ times larger than $\tau_{bb}(0,t)_B$.

To verify the formulas (332) through (334), the numerical simulations of this random walk property were performed, and the results are shown in Figure 33. The conditions used in the simulations are as follows; $\alpha_+ = 0.3$, $\alpha_- = 0.2$, $p^{(V)} = 0.45$, $N_x = N_y = 2$, $v = 1$ and $t_0 = 1$. Clearly, the numerical results are in agreement with the analytical results.

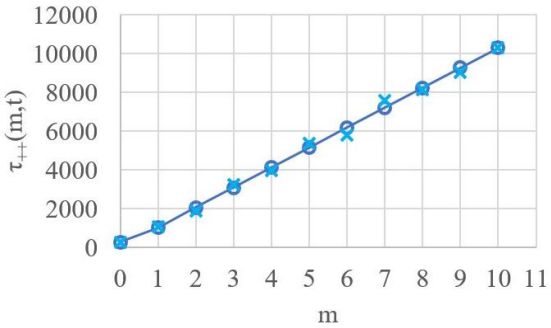


Figure 33. The dependence of the distance m of the considered site on the conditional mean first-passage time $\tau_{++}(m,t)$ for given time $t = 10^5$. The circles and the crosses represent the analytical and the numerical results respectively.

The resemble between the unbiased random walk on the ladder and the unbiased DRWFG on the branched lattice B can also be found in the asymptotic

form of the expected number $\langle S\rangle(t)$ of distinct major sites visited at large times. As the important parameters are found, the expected number can be calculated from

$$\langle S\rangle(t) \sim \frac{4}{\Gamma(1+\nu/2)}\sqrt{\frac{\langle\alpha^*\rangle}{G}}\left(\frac{t}{t_0}\right)^{\frac{\nu}{2}}. \tag{335}$$

As compared with the result $\langle S\rangle(t)_B$ in equation (261) of the unbiased DRWFG on the branched lattice, the result in equation (335) is double of $\langle S\rangle(t)_B$. It is because, in each unit cell of the ladder, there are two major sites to be discovered.

This completes our analysis of the basic properties of the vertically symmetrical random walk on ladders. From this model, we can see that many basic properties are related to the diffusion coefficient D which can be considered as the weighted average of the diffusion coefficients $D_{\pm}$ of the random walk on the + and the – rails, $D = D_+\pi_+ + D_-\pi_-$ where $D_{\pm} \equiv \frac{(N_x+1)^2}{\Gamma(1+\nu)Gt_0^{\nu}}\alpha_{\pm}^*$. Therefore, to a certain extent, the formalism for the random walk on ladders may be used to investigate transport properties of models for media possessing two diffusivities. As an example, in the following section, we will discuss the relation between this random walk model and the recognition between a DNA-binding protein and its specific target DNA sequence.

5.5 Protein diffusion along DNA

As introduced in Subsection 1.4.3, Krepel and Levy [45] have numerically demonstrated that the protein recognizes its DNA target through a combination of two types of diffusions, i.e., “one-dimensional” diffusion, the protein “slides” or “hops” along the DNA, and “three-dimensional” diffusion, the protein may move away from the DNA and diffuse into 3D bulk. The dependence of the volume fraction occupied by the crowding particle on the search time is of their interest.

We find that if we consider a protein as a walker, the protein motions on DNA and in 3D bulk as the walker motions in the + and the – rails, then we can show that, in certain limit, the search time is inversely proportional to the square root of the volume fraction.

To see this, in the first place, let us set $N_x, N_y = 0$ and $\nu = 1$ because the walker possibly leaves or return to DNA strand at any step and the transport is normal diffusion. Then we associate the probabilities of leaving from and returning to DNA strand with the transition probabilities β_+ and β_- respectively. To note that the relation between the transition probability β_- and the volume fraction φ occupied by the crowding particles is the important relation. Although we do not know the exact form of the relation, to a certain extent, it is reasonable to assume that they are a linear function of each other when the volume fraction is small. From the preceding argument, let assume that

(i) the volume fraction φ is small,

(ii) the probability β_+ is independent of the volume fraction φ,

(iii) the probability β_- is very small comparing to the probability β_+

(iv) the relation between β_- and φ is linear, i.e., $\beta_- = \beta_0 + f\varphi$ where β_0 is the probability of returning to DNA strand without any crowding particle and f is a certain constant.

Combining these assumptions with equation (299) leads us to the expression of diffusion coefficient in the linear function of φ,

$$D = b(\varphi + \varphi_0) \tag{336}$$

where $b = \frac{1}{2t_0}\frac{(1-\beta_+)}{\beta_+} f$ and $\varphi_0 = \frac{1}{2b} + \frac{1}{f}\beta_0$. Since the search time is the mean time required for the searching protein to approach the target site by predefined time, which is equivalent to the conditional mean first-passage time to a given major site by certain time, we can determine the dependence of the volume fraction occupied by the crowding particle on the search time from equation (336) together with equations (299) and (334),

$$\tau(m,t,\varphi) \sim \frac{c(m,t)}{\sqrt{\varphi + \varphi_0}} \tag{337}$$

where $c(m,t)$ is a certain function of the distance m of the target site from the starting site and the observed time t. If the variables m and t are fixed, then the values of φ_0 and $c(m,t)$ can be found from experimental results by the following

equations $\varphi_0 = \left(\left(\frac{\tau(m,t,0)}{\tau(m,t,\varphi')} \right)^2 - 1 \right)^{-1} \varphi'$ and $c(m,t) = \tau(0) \sqrt{\left(\left(\frac{\tau(m,t,0)}{\tau(m,t,\varphi')} \right)^2 - 1 \right)^{-1}} \varphi'$ where φ' is another volume fraction which is not equal to zero.

Figure 34 shows that equation (337) is in agreement with numerical results of Krepel and Levy at low volume fractions, where φ_0 and $c(m,t)$ were determined by the search times from the numerical simulation at $\varphi = 0$ and $\varphi = 0.05$. However, at high volume fractions, the analytical results give less time.

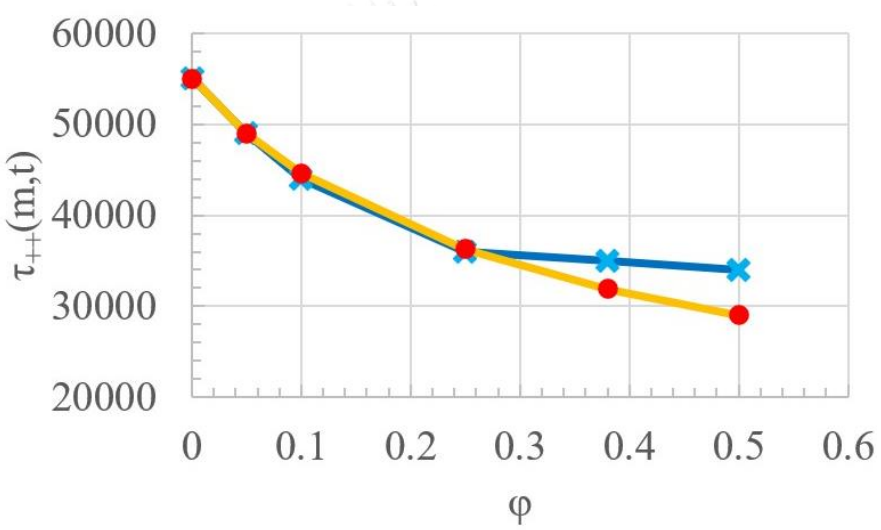


Figure 34. The graphs of the numerical results (blue crosses) and our analytical results (red dots)

5.6 Conclusion

We have considered some basic properties of the random walk on ladder lattices, consisting of two parallel rails (1-d infinite lattices) periodically connected to each other with rungs (1-d finite lattices). We could express the explicit forms of the generating function $P_{ab}(m;\xi)$ only in the cases of the horizontally and the vertically symmetrical random walks because the full analysis is involved with the factorization of the fourth degree complex polynomial function.

We found that most of the basic properties of these kind of random walks are identical to the DRWFGs on branched lattices except for a renormalization of

coefficients and for the probability of ever reaching a given major site for the biased random walk.

For the unbiased random walk on the ladder lattices, the diffusion coefficient can be considered as the weighted average of the diffusion coefficients $D_{\pm}$ of the random walk on the + and the – rails, i.e.,

$$D = D_{+}\pi_{+} + D_{-}\pi_{-} \tag{338}$$

where $D_{\pm} \equiv \frac{\left(N_x+1\right)^2}{\Gamma\left(1+v\right)Gt_0^v}\alpha_{\pm}^{*}$. The asymptotic behavior of various other properties of the random walk are governed by this diffusion coefficient. For instance, the probability of returning to the starting site,

$$P_{bb}\left(0,t\right) \sim \frac{\pi_b\left(N_x+1\right)}{2G\Gamma\left(1-\frac{v}{2}\right)\sqrt{\Gamma\left(1+v\right)t_0^v D}}\left(\frac{t}{t_0}\right)^{-v/2} \tag{339}$$

and the expected number of distinct major sites visited at large times,

$$\left\langle S\right\rangle\left(t\right) \sim \frac{4\sqrt{\Gamma\left(1+v\right)t_0^v D}}{\left(N_x+1\right)\Gamma\left(1+v/2\right)}\left(\frac{t}{t_0}\right)^{\frac{v}{2}}. \tag{340}$$

From these results, roughly speaking, if the diffusion coefficient of the walker increases, it is more likely to find new major sites but less likely to return to the starting site.

To a certain extent, the formalism for the random walk on ladder lattices may be used to investigate transport properties of models for media possessing two diffusivities. As an example, we applied our results to the problem of recognition between a DNA-binding protein and its specific target DNA sequence.

6

Random walks on cylindrical lattices

In this chapter we make a direct extension to multi-major-site models of the method used in the previous chapter for the two-major-site model. For sake of simplicity, we concentrate on multi-major-site structures, called cylindrical lattices and shown in Figure 35, whose major sites in each unit cell are equivalent. It is worth stressing that this model may be extended to more general models if desired. The first two moments of biased and unbiased random walks on the cylindrical lattices can be calculated without any difficulty. Nevertheless, for the other basic properties, we limit ourselves to the unbiased random walks due to the difficulty of mathematical problems for the case of the biased random walks.

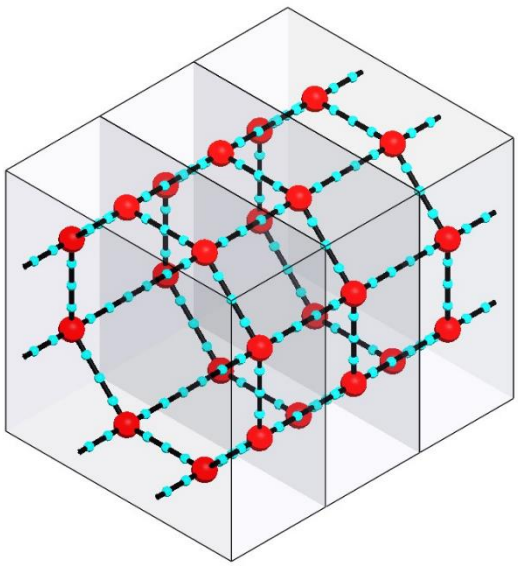


Figure 35. A schematic of a cylindrical lattice. Major sites and minor sites are represented by red and blue spheres respectively.

6.1 Model

A cylindrical lattice is a quasi-1d infinite structure whose each unit cell contains $N_M \geq 3$ different major sites on a circular ring with a N_y+1-length 1-d lattice between two nearest major sites. Each major site is connected to its equivalent site in the next unit cell by a N_x+1-length 1-d lattice. There are thus $N = N_M\left(N_x+N_y+1\right)$ different sites in each unit cell. A schematic of a cylindrical lattice is shown in Figure 35. Without loss of generality, the distance between neighboring sites is set to be unity.

Here, we will also use the same coordinate system established in Chapter 2. The origin O is placed at a certain major site within a unit cell, labelled the 0th unit cell. Unit cells and sites within each unit cell are labelled by letters m and a, respectively. The position of the major site, which is an equivalent site to the origin, within the mth unit cell is thus given by $m\left(N_x+1\right)\hat{x}$. The relative positions of sites within the unit cell to this major site are denoted by $\vec{r}_1,\vec{r}_2,\vec{r}_3,...,\vec{r}_N$ where the vectors $\vec{r}_1,\vec{r}_2,\vec{r}_3,...,\vec{r}_{N_M}$ are for major sites and the remaining vectors are for minor sites. The vector $\vec{r}_1=0$ is for the major site itself. For the relative positions of major sites, a major site $\vec{r}_i$ is the nearest major site to major sites $\vec{r}_{i+1}$ and $\vec{r}_{i-1}$ for $i=1,2,3,...,N_M$ with $\vec{r}_0=\vec{r}_{N_M}$ and $\vec{r}_{N_M+1}=\vec{r}_1$. Accordingly, the position of the ath site in the mth unit cell indicated by the vector $\vec{x}_{m,a}$ may be represented as $\vec{x}_{m,a}=m\left(N_x+1\right)\hat{x}+\vec{r}_a$ where $a=1,2,3,...,N$ or $\left(x_{m,a},y_{m,a},z_{m,a}\right)$.

A walker located at a major site may jump to the right, left, up or down neighboring sites with probabilities α, γ, β and β respectively. These transition probabilities satisfy the normalization condition, $\alpha+\gamma+2\beta=1$. When the walker is at a minor site on a N_y+1-length 1-d lattice, it can jump to the up or down neighboring sites with probability 0.5. On the other hand, if the walker is at a minor site on a N_x+1-length 1-d lattice, it may jump to the right and left neighboring sites with probabilities $p^{(H)}$ and $q^{(H)}=1-p^{(H)}$ respectively.

6.2 Results and discussion

For this model, every major site is equivalent to each other in the sense that when a walker is at any major site, it obeys the same set of transition probabilities. Accordingly, the generating functions $\bar{p}_{ij}(k;\xi)$ of the multi-step transition probabilities satisfy the following relations: $\bar{p}_{ij}(k;\xi)=\bar{p}_{i-1\,j-1}(k;\xi)$ for $i,j=1,2,3,\ldots,N_M$ where $\bar{p}_{0j}(k;\xi)=\bar{p}_{N_M j}(k;\xi)$, $\bar{p}_{i0}(k;\xi)=\bar{p}_{iN_M}(k;\xi)$ and $\bar{p}_{00}(k;\xi)=\bar{p}_{N_M N_M}(k;\xi)$. From the restriction that only nearest major sites are directly connected to each other by finite 1-d lattices, we have $\bar{p}_{i1}(k;\xi)=0$ for $i=3,4,5,...,N_M-1$. Altogether, the matrix $\bar{\mathrm{p}}(k;\xi)$ can be written as

$$\bar{\mathrm{p}}(k;\xi)=\begin{bmatrix} \bar{p}_{11}(k;\xi) & \bar{p}_{21}(k;\xi) & \cdots & 0 & \bar{p}_{21}(k;\xi) \\ \bar{p}_{21}(k;\xi) & \bar{p}_{11}(k;\xi) & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \bar{p}_{11}(k;\xi) & \bar{p}_{21}(k;\xi) \\ \bar{p}_{21}(k;\xi) & 0 & \cdots & \bar{p}_{21}(k;\xi) & \bar{p}_{11}(k;\xi) \end{bmatrix} \tag{341}$$

where $\bar{p}_{11}(k;\xi)\equiv\gamma^*(\xi)e^{-i(N_x+1)k}+\Sigma(\xi)+\alpha^*(\xi)e^{i(N_x+1)k}$ and $\bar{p}_{21}(k;\xi)\equiv\beta^*(\xi)$. The equivalence of major sites leads us to $\pi_1(k;\xi)=\ldots=\pi_{N_M}(k;\xi)$ with $\pi_1(k;\xi)=\frac{1}{N_M}\left(\bar{p}_{11}(k;\xi)+2\bar{p}_{21}(k;\xi)\right)$, which gives the limits

$$\pi_i=\frac{1}{N_M} \tag{342}$$

for $i=1,2,3,...,N_M$, and the eigenfunction

$$E_1(k;\xi)=\sum_{i=1}^{N_M}\bar{p}_{ij}(k;\xi) \tag{343}$$

for any $j=1,2,3,\ldots,N_M$. Furthermore, from the definition of $\bar{p}_{ij}(k;\xi)$, the sum $\sum_{i=1}^{N_M}\bar{p}_{ij}(k;\xi)$ can be written in the form

$$\sum_{i=1}^{N_M}\bar{p}_{ij}(k;\xi)=\gamma^*(\xi)e^{-ik(N_x+1)}+\Sigma(\xi)+2\beta^*(\xi)+\alpha^*(\xi)e^{ik(N_x+1)} \tag{344}$$

where, for $\lambda_\pm(p;\xi)=\frac{1\pm\sqrt{1-4p(1-p)\xi^2}}{2p\xi}$,

$$\alpha^*(\xi)=\xi\alpha\left(\frac{\lambda_+\left(p^{(H)};\xi\right)-\lambda_-\left(p^{(H)};\xi\right)}{\lambda_+^{N_x+1}\left(p^{(H)};\xi\right)-\lambda_-^{N_x+1}\left(p^{(H)};\xi\right)}\right),$$

$$\gamma^*(\xi)=\xi\gamma\left(\frac{\lambda_+\left(q^{(H)};\xi\right)-\lambda_-\left(q^{(H)};\xi\right)}{\lambda_+^{N_x+1}\left(q^{(H)};\xi\right)-\lambda_-^{N_x+1}\left(q^{(H)};\xi\right)}\right),$$

$$\beta^*(\xi)=\xi\beta\left(\frac{\lambda_+(0.5;\xi)-\lambda_-(0.5;\xi)}{\lambda_+^{N_y+1}(0.5;\xi)-\lambda_-^{N_y+1}(0.5;\xi)}\right),$$

$$\Sigma(\xi)=\quad\xi\alpha\left(\frac{\lambda_+^{N_x}\left(q^{(H)};\xi\right)-\lambda_-^{N_x}\left(q^{(H)};\xi\right)}{\lambda_+^{N_x+1}\left(q^{(H)};\xi\right)-\lambda_-^{N_x+1}\left(q^{(H)};\xi\right)}\right)+$$

$$\xi\gamma\left(\frac{\lambda_+^{N_x}\left(p^{(H)};\xi\right)-\lambda_-^{N_x}\left(p^{(H)};\xi\right)}{\lambda_+^{N_x+1}\left(p^{(H)};\xi\right)-\lambda_-^{N_x+1}\left(p^{(H)};\xi\right)}\right)+.$$

$$\xi 2\beta\left(\frac{\lambda_+^{N_y}(0.5;\xi)-\lambda_-^{N_y}(0.5;\xi)}{\lambda_+^{N_y+1}(0.5;\xi)-\lambda_-^{N_y+1}(0.5;\xi)}\right)$$

Since the subsequent results are very similar to those in the previous chapters, we condense the discussion here. From the finiteness of the size of the connected networks, it can be shown that a random walk on a cylindrical lattice is a DRWFG,

$$1-E_1(0;\xi)\sim(1-\xi)G, \tag{345}$$

which gives

$$c_1=G \text{ and } d_H=1, \tag{346}$$

where

$$G=\alpha\tau_\alpha\left(p^{(H)},N_x+1\right)+\gamma\tau_\gamma\left(p^{(H)},N_x+1\right)+2\beta\tau_\alpha\left(0.5,N_y+1\right)+1. \tag{347}$$

Let us now calculate the effective velocity ϑ and the diffusion coefficient D by substituting the entries $\bar{p}_{ab}\left(k;1^-\right)$ into equations (182) and (183). We find that the effective velocity and the diffusion coefficient are in the same form as those for DRWFGs on branched lattices (see equations (225) and (226)),

$$\vartheta=\frac{\left(N_x+1\right)\left(\alpha^*-\gamma^*\right)}{\Gamma(1+\nu)Gt_0^\nu} \tag{348}$$

and

$$D=\frac{\left(N_x+1\right)^2\alpha^*}{\Gamma(1+\nu)Gt_0^\nu}. \tag{349}$$

As we have encountered in the previous models, to completely determine the basic random walk properties for a given major site, the explicit forms of the generating functions $P_{ab}(m;\xi)$ are desired. They can be found from

$$P_{ab}(m;\xi)=\frac{1}{2\pi i}\oint_{C}\frac{\mathrm{adj}\left[\mathrm{I}-\bar{\mathrm{p}}(k(z);\xi)\right]_{ab}}{\det\left[\mathrm{I}-\bar{\mathrm{p}}(k(z);\xi)\right]}z^{-m}\frac{dz}{z}.$$

For any number N_M of major sites in each unit cell, we can express the close form of the determinate of the matrix $\mathrm{I}-\bar{\mathrm{p}}(k;\xi)$ (see Appendix 14),

$$\det\left[\mathrm{I}-\bar{\mathrm{p}}(k;\xi)\right]=\prod_{i=1}^{N_M}\left(1-E_i(k;\xi)\right) \tag{350}$$

where $E_i(k;\xi)=\bar{p}_{11}(k;\xi)+2\cos\left(\frac{2\pi(i-1)}{N_M}\right)\bar{p}_{21}(k;\xi)$, but the close form of the adjugate matrix is still a mystery.

Fortunately, for unbiased random walks, to determine the asymptotic forms of the basic properties for a given major site, only the information of the singular part $\left(z^{(1)}(\xi)\right)^{|m|}P_{ab}^{(1)}(\xi)$ of the generating function $P_{ab}(m;\xi)=\sum_{i=1}^{N_M}\left(z^{(i)}(\xi)\right)^{|m|}P_{ab}^{(i)}(\xi)$, i.e., the asymptotic forms of the terms $P_{bb}^{(1)}(\xi)$ and $\left(z^{(1)}(\xi)\right)'$, is required. From equation (350), we can show that (see Appendix 15)

$$P_{bb}^{(1)}(\xi)\sim\frac{\pi_b}{2\sqrt{\alpha^* G}}(1-\xi)^{-\frac{1}{2}}$$

and

$$\left(z^{(1)}(\xi)\right)'\sim\frac{1}{2}\sqrt{\frac{G}{\alpha^*}}(1-\xi)^{-\frac{1}{2}}$$

which lead to

$$c_2=\frac{1}{2\sqrt{\alpha^* G}}, \tag{351}$$

$$c_3=\frac{1}{2}\sqrt{\frac{G}{\alpha^*}}. \tag{352}$$

Again, we can substitute equations (346) – (349), (351) and (352) into equations (184) through (198) and find the basic random walk properties. As compared with the unrestricted 1-d lattice model, we find that the additional structure does not affect the exponents but does have a great impact on the coefficients. Figure 36 shows the numerical results (symbols) of the certain basic

properties compared with the analytical results (solid lines) under the same conditions, i.e., $\gamma = \alpha = 0.3$, $p^{(H)} = 0.5$, $N_x = 3$, $N_y = 2$, $v = t_0 = 1$ and $N_M = 3,4,5$ with $P_0 \equiv \left[2\sqrt{\alpha^* G} N_M \Gamma(1-v/2)\right]^{-1}$, $\tau_0 \equiv \frac{v t_0 |m| \sqrt{G/\alpha^*}}{2\Gamma(2-v/2)}$ and $S_0 \equiv \frac{2N_M \sqrt{\alpha^*/G}}{\Gamma(1+v/2)}$.

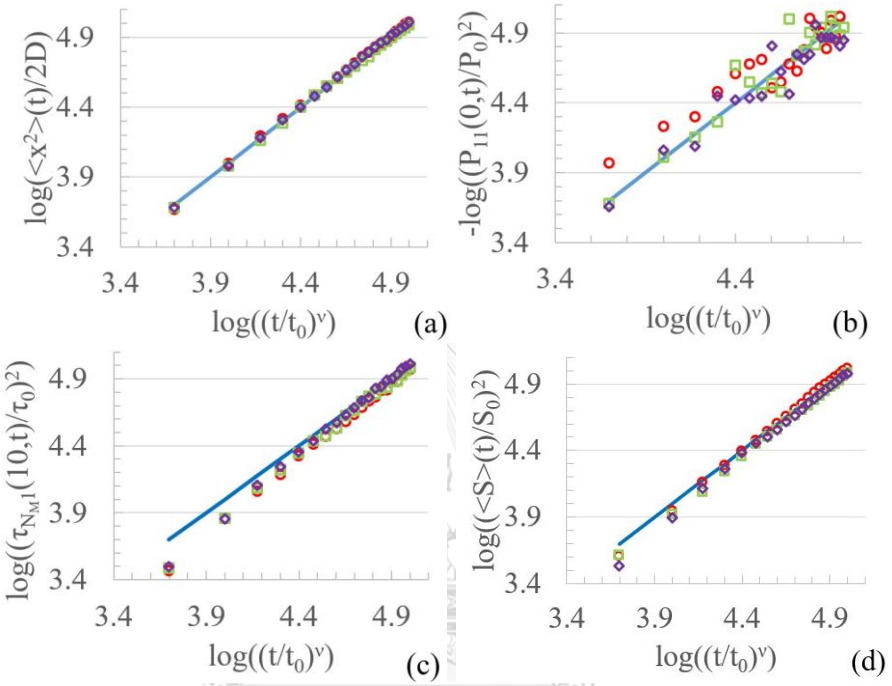


Figure 36. The numerical results of the second moment (a), the probability of return to the starting site (b), the conditional mean first-passage time to a given major site by time t (c) and the expected number of distinct major sites visited at large times (d) compared with the analytical results.

Before ending this chapter, let us digress to make a comment on the mathematically interesting result related to equation (350). From equation (108), we have

$$\frac{1}{N_M} = \frac{\left[\mathrm{adj}\left(\mathrm{I}-\bar{\mathrm{p}}\left(0;1^-\right)\right)\right]_{11}}{\prod_{i=2}^{N_M}\left(1-E_i\left(0;1^-\right)\right)} \tag{353}$$

where $\pi_1 = 1/N_M$ was used. Since we can show that (see Appendix 14)

$$\left[\mathrm{adj}\left(\mathrm{I}-\bar{\mathrm{p}}\left(0;1^-\right)\right)\right]_{11} = N_M \left(\beta^*\right)^{N_M - 1}, \tag{354}$$

$$\prod_{n=2}^{N_M}\left(1-E_n\left(0;1^-\right)\right)=\left(2\beta^*\right)^{N_M-1}\prod_{i=2}^{N_M}\left(1-2\cos\left(\frac{2\pi\left(i-1\right)}{N}\right)\right), \tag{355}$$

after substituting equations (354) and (355) into equation (353) and rearranging, we obtain the finite product of cosine functions

$$\prod_{i=1}^{N_M-1}\left(1-\cos\left(\frac{2\pi i}{N_M}\right)\right)=\frac{N_M^2}{2^{N_M-1}}. \tag{356}$$

6.3 Nonlinear transport in quasi-1d materials

Let us close the chapter by the discussion of nonlinear transport in quasi-1d materials in the random walk point of view. As discussed in Subsection 1.4.5, the power-law dependence of the current on bias voltage,

$$I\propto V^{1+\eta}, \tag{357}$$

has been observed in a great number of quasi-1d materials, e.g., single-wall carbon nanotubes [64], at low temperatures. In certain limit, this phenomenon may be able to be transcribed into a random walk on quasi-1d infinite structures via the following assumptions:

(i) The structural features of a quasi-1d material can be reproduced by a quasi-1d infinite structure whose the effective dimension is unity, $d_H=1$.

(ii) The motion of an individual electron in the quasi-1d material at low temperatures can be described by the separable continuous-time random walk, given that a walker started at a certain unit cell associating with one of bias probes.

(iii) The effect of impurity or disorder in the quasi-1d material is attributed to the behavior of the PDF $\psi\left(t\right)$ of waiting time.

(iv) The bias voltage is proportional to the difference of the multi-step transition probabilities along the direction of the structure axis, i.e.,

$$V\propto\left|\alpha^*-\gamma^*\right|. \tag{358}$$

(v) The measured current is the space average of the conduction current in the material, which is proportional to the first moment of the walker location along the structure axis evaluated at the time equal to the

conditional mean first-passage time $\tau\left(m,t^*\right)$ to the unit cell associating with the other probe before the observing time t^*,

$$I \propto \left.\frac{d\langle x\rangle(t)}{dt}\right|_{\tau\left(m,t^*\right)} \tag{359}$$

where the distance m associates with the distance between two probes. To note that here we do not focus on the structural dependence of the relation (357) so, for clarity and simplicity, let us use the cylindrical structure.

Before we move on, from the assumption (v), the conditional mean first-passage time $\tau(m,t)$ to any major sites in the m th unit cell by time t need to be determined. First let us consider the generating function $P(m;\xi)$ of the probability that the walker is at any major sites in the m th unit cell at the n th step. From equation (79), if only major sites are taken into account, we have

$$P_{ab}(m;\xi)=\delta_{m,0}\delta_{a,b}+\sum_{c=1}^{N_M}\sum_{\Delta m=-1}^{1}p_{ac}(\Delta m;\xi)P_{cb}(m-\Delta m;\xi). \tag{360}$$

Then we sum this equation over all possible starting and arriving major sites,

$$P(m;\xi)=\delta_{m,0}+\sum_{\Delta m=-1}^{1}p(\Delta m;\xi)P(m-\Delta m;\xi) \tag{361}$$

where $P(m;\xi)\equiv\frac{1}{N_M}\sum_{a=1}^{N_M}\sum_{b=1}^{N_M}P_{ab}(m;\xi)$, $p(\Delta m;\xi)\equiv\sum_{a=1}^{N_M}p_{ac}(\Delta m;\xi)$. We have assumed that the probabilities of starting at any major sites in the 0 th unit cell are the same. Note that, from equation (344),

$$p(\Delta m;\xi)=\gamma^*(\xi)\delta_{\Delta m,-1}+\left(\Sigma(\xi)+2\beta^*(\xi)\right)\delta_{\Delta m,0}+\alpha^*(\xi)\delta_{\Delta m,1}. \tag{362}$$

It should be noticed that this is analogous to the one-major-site problem (see, e.g., equation (221)) so we can employ the results found in Chapter 4 to determine the basic properties of the random walks on cylindrical lattices for given unit cell, on regardless of major sites. From equation (260), we therefore have

$$\tau(m\neq 0,t)\sim\left|\frac{mG}{\alpha^*-\gamma^*}\right|\frac{vt_0}{\Gamma(2-v)}\left(\frac{t}{t_0}\right)^{1-v} \tag{363}$$

for appropriate associating parameters. Consequently, this result and the previous assumptions yield

$$I\propto\frac{Lv}{Gt_0\Gamma(1+v)}\left(\frac{vmG}{\Gamma(2-v)}\right)^{v-1}\left(\frac{t^*}{t_0}\right)^{-(1-v)^2}\left(\alpha^*-\gamma^*\right)^{2-v}. \tag{364}$$

When all variables except $\alpha^* - \gamma^*$ are fixed, this result is in agreement with the experimental result given in equation (357) where

$$\eta = 1 - \nu . \tag{365}$$

This implies that if the exponent η does not vanish, then the electron transport is anomalous. Otherwise, it is normal, and the corresponding quasi-1d material behaves as an ohmic resistor, $I \propto V$.

In our model point of view, at an intermediate temperature, the conditional mean time that an electron starting from one probe travels to the other decays as temperature increases. It may be approximated by

$$\tau\left(m, t^*\right) \approx a\left(b + \frac{kT}{\langle U \rangle}\right)^{-c} \tag{366}$$

where a, b, c are fitting parameters, when other variables, e.g., the bias voltage and the distance between probes, are fixed. To see this, equation (363) and the analysis of Bendler and Shlesinger for parameter ν, i.e., $\nu \equiv kT/\langle U \rangle$ (see Section 2.3), need to be taken into account. Figure 37 shows the plots of $\tau\left(m, t^*\right)$ in equation (363) as $kT/\langle U \rangle$ is solely varied, and of its approximation from equation (366) with $t^* = \lambda_0 = 1000$, $a = 0.4$, $b = 0.38$, $c = 7$.

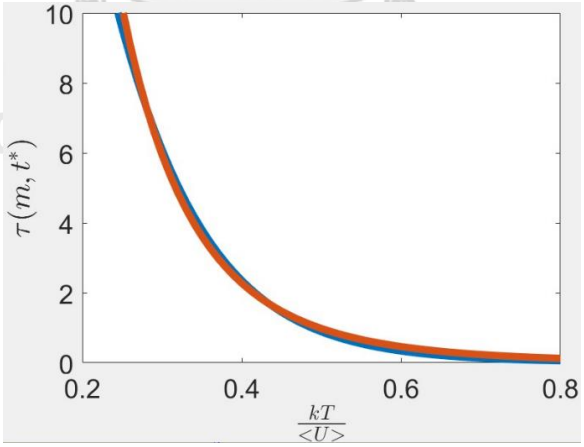


Figure 37. The plots of the conditional mean first-passage time $\tau\left(m, t^*\right)$ (blue) and of its approximation (orange).

7

Summary

This PhD thesis addressed the study of random walks on quasi-1d infinite structures, investigating basic statistical properties of the random walks through the generating function formalism. Our work can be briefly summarized as follows.

In **Chapter 2**, we developed a formalism by mainly employing the concepts of the Chapman–Kolmogorov equation, the generating functions, the Fourier-Laplace transform and the irreducible Markov chains. From the developed formalism, we could establish the systematic method called the generating function formalism (GFF) for obtaining the asymptotic behavior of basic statistical properties of the random walks including the first and the second moments of the walker location along the structure axis at large times, the probability of return to the starting site at large times, the probability of ever reach a given major site, the conditional mean first-passage time to a given major site and the expected number of distinct major sites visited at large times. The adoption of GFF to certain quasi-1d infinite structure models is solely required the mesoscopic characteristics of the corresponding random walk, i.e., the probability of waiting time and the multi-step transition probabilities between two "major" sites. As the first adoption of GFF in this thesis, in **Chapter 3**, we applied it to the well-known problem, a random walk on a 1-d perfect lattice. The obtained results showed a perfect agreement with the well-known results.

In **Chapter 4**, as the first non-trivial application of GFF, we considered random walks on branched lattices. We found that the spectral dimension d_H of a perfect 1-d lattice is changed from unity to $d_H = 1 + \frac{1}{2} d'_H$ when fractals with the spectral dimension $0 < d'_H < 2$ are periodically attached to sites on the lattice. This led us to various transport behavior of a walker along the structure axis depending

on the localized transition on the attached fractals. We pointed out that when 1-d lattices, $d'_H = 1$, are attached to sites, the corresponding random walk model is either the so-called comb model or its generalization, a sparse comb model, depending on the periodicity or the sparsity of the attachment. The sparsity dependence of the random walk properties was studied, and several interesting results were found.

In **Chapter 5**, we studied random walks on ladder lattices. Unlike a 1-d perfect lattice and a branched lattice, a ladder lattice primarily consists of two parallel 1-d lattices, which are periodically connected to each other with finite 1-d lattices. We showed how the localized transports of the walker on these primary axes contribute to its basic random walk properties. We found that most of the basic properties are identical to those for a perfect 1-d lattice except for a rescaling of coefficients and for the probability of ever reach a given major site. We showed that even the considered major site is located in the same direction of bias, the probability of ever reach that site is always less than unity. In addition, from the resemble of the ladder lattice model and a two-state random walk on a 1-d lattice, which may be used to investigate transport properties of models for media possessing two diffusivities, we thus discussed the transcription of the problem of the DNA search by a protein into the language of the ladder lattice model.

In **Chapter 6**, we studied random walks on cylindrical lattices, the structures that consist of many parallel 1-d lattices periodically connected to each other with finite 1-d lattices. For general cases, we could determine the first and the second moments of a walker location along the structure axis at large times by employing GFF without any difficulty. However, according to the mathematical difficulty, the other random walk properties were considered only in the cases that the walker is “unbiased” along the structure axis, i.e., the first moment vanishes. From the obtained results together with the assumption that the cylindrical lattice model can reproduce certain features of transport processes in quasi-1d materials, e.g., nanowires and single-wall carbon nanotubes, we could relate the non-ohmic current-voltage characteristics in quasi-1d materials to the anomalous transport of the random walker on the quasi-1d lattices.

APPENDICES

Appendix 1

From equation (69), the Laplace transform

$$\wp^*\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right)\equiv\int_0^\infty\wp\left(\vec{x}_{m,a},t\,|\,\vec{x}_{0,b}\right)e^{-st}dt \tag{367}$$

can be expressed as

$$\wp^*\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right)=\int_0^\infty e^{-st}\int_0^t\left(\sum_{n=0}^\infty\wp\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_n\psi\left(t'\right)_n\right)\Psi\left(t-t'\right)dt'dt\,. \tag{368}$$

It is assumed that the resulting integral is identical to term-by-term integration,

$$\wp^*\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right)=\sum_{n=0}^\infty\wp\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_n\left(\int_0^\infty e^{-st}\left(\int_0^t\psi\left(t'\right)_n\Psi\left(t-t'\right)dt'\right)dt\right). \tag{369}$$

After using the convolution theorem of the Laplace transform, we have

$$\wp^*\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right)=\sum_{n=0}^\infty\wp\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_n\left(\int_0^\infty e^{-st}\psi\left(t\right)_n dt\right)\left(\int_0^\infty e^{-st}\Psi\left(t\right)dt\right). \tag{370}$$

Use the definitions of the Laplace transform and of $\Psi\left(t\right)$, we obtain

$$\wp^*\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right)=\sum_{n=0}^\infty\wp\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_n\psi^*\left(s\right)_n\left(\int_0^\infty e^{-st}\left(1-\int_0^t\psi\left(t'\right)dt'\right)dt\right). \tag{371}$$

Find the Laplace transform of term in the parentheses,

$$\wp^*\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right)=\sum_{n=0}^\infty\wp\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_n\psi^*\left(s\right)_n\left(\frac{1}{s}-\frac{\psi^*\left(s\right)}{s}\right). \tag{372}$$

Now, let us consider the Laplace transform $\psi^*\left(s\right)_n$. From its definition, we have

$$\psi^*\left(s\right)_n=\int_0^\infty e^{-st}\left(\int_0^t\psi\left(t-t'\right)_{n-1}\psi\left(t'\right)dt'\right)dt\,. \tag{373}$$

After applying the convolution theorem to this, we obtain

$$\psi^*\left(s\right)_n=\psi^*\left(s\right)_{n-1}\psi^*\left(s\right), \tag{374}$$

and, as $\psi^*\left(s\right)_0=1$, it is straightforward that

$$\psi^*\left(s\right)_n=\left(\psi^*\left(s\right)\right)^n. \tag{375}$$

Therefore, equation (372) can be expressed as

$$\wp^*\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right)=\left(\frac{1-\psi^*\left(s\right)}{s}\right)\sum_{n=0}^\infty\wp\left(\vec{x}_{m,a}\,|\,\vec{x}_{0,b}\right)_n\left(\psi^*\left(s\right)\right)^n \tag{376}$$

or

$$\wp^*\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right)=\left(\frac{1-\psi^*\left(s\right)}{s}\right)\wp\left(\vec{x}_{m,a};\psi^*\left(s\right)|\,\vec{x}_{0,b}\right). \tag{377}$$

Appendix 2

If we put equation (79) into

$$\tilde{\wp}\left(k,\vec{r}_a;\xi\,|\,\vec{x}_{0,b}\right)=\sum_{m=-\infty}^{\infty}e^{ikmL}\wp\left(\vec{x}_{m,a};\xi\,|\,\vec{x}_{0,b}\right), \tag{378}$$

we have

$$\tilde{\wp}\left(k,\vec{r}_a;\xi\,|\,\vec{x}_{0,b}\right)=\sum_{m=-\infty}^{\infty}e^{ikmL}\left\{\delta_{m,0}\delta_{a,b}+\sum_{c=1}^{N_M}\sum_{\Delta m=-1}^{1}p\left(\vec{r}_a,-\Delta mL\hat{x}+\vec{r}_c;\xi\right)P_{cb}\left(m-\Delta m;\xi\right)\right\}. \tag{379}$$

It is immediate that

$$\tilde{\wp}\left(k,\vec{r}_a;\xi\,|\,\vec{x}_{0,b}\right)=\delta_{a,b}+\sum_{m=-\infty}^{\infty}\sum_{c=1}^{N_M}\sum_{\Delta m=-1}^{1}e^{ikmL}p\left(\vec{r}_a,-\Delta mL\hat{x}+\vec{r}_c;\xi\right)P_{cb}\left(m-\Delta m;\xi\right). \tag{380}$$

After multiplying and dividing certain terms to this equation and interchanging the order of summation, it becomes

$$\tilde{\wp}\left(k,\vec{r}_a;\xi\,|\,\vec{x}_{0,b}\right)= \\ \delta_{a,b}+\sum_{c=1}^{N_M}\sum_{\Delta m=-1}^{1}e^{ik\Delta mL}p\left(\vec{r}_a,-\Delta mL\hat{x}+\vec{r}_c;\xi\right)\sum_{m=-\infty}^{\infty}e^{ik(m-\Delta m)L}P_{cb}\left(m-\Delta m;\xi\right). \tag{381}$$

From the definitions of the Fourier transform and

$\bar{p}\left(k,\vec{r}_a,\vec{r}_c;\xi\right)\equiv\sum_{\Delta m=-1}^{1}e^{ik\Delta mL}p\left(\vec{r}_a,-\Delta mL\hat{x}+\vec{r}_c;\xi\right)$, we have, for $a=1,2,3,...,N$,

$$\tilde{\wp}\left(k,\vec{r}_a;\xi\,|\,\vec{x}_{0,b}\right)=\delta_{a,b}+\sum_{c=1}^{N_M}\bar{p}\left(k,\vec{r}_a,\vec{r}_c;\xi\right)\tilde{P}_{cb}\left(k;\xi\right). \tag{382}$$

For $a=1,2,3,...,N_M$, this becomes

$$\tilde{P}_{ab}\left(k;\xi\right)=\delta_{a,b}+\sum_{c=1}^{N_M}\bar{p}_{ac}\left(k;\xi\right)\tilde{P}_{cb}\left(k;\xi\right) \tag{383}$$

with $\bar{p}_{ac}\left(k;\xi\right)\equiv\sum_{\Delta m=-1}^{1}e^{ik\Delta mL}p_{ac}\left(\Delta m;\xi\right)$ and $p_{ac}\left(\Delta m;\xi\right)\equiv p\left(\vec{r}_a,-\Delta mL\hat{x}+\vec{r}_c;\xi\right)$.

Appendix 3

For a given $N\times N$ matrix A, using the definition of an eigenvalue, we can show that

$$\det\left(E\mathrm{I}-\mathrm{A}\right)=\prod_{n=1}^{N}\left(E-E_n\right) \tag{384}$$

where E_n is an eigenvalue of the matrix A and E is any number. Therefore, if we choose $E=1$, we have

$$\det\left(\mathrm{I}-\mathrm{A}\right)=\prod_{n=1}^{N}\left(1-E_n\right). \tag{385}$$

Appendix 4

If A is an $N \times N$ matrix that satisfies the following conditions:

1. $\sum_{i=1}^{N} A_{ij} = 0$ for $j = 1, 2, 3, ..., N$
2. There exists a eigenvector $\pi \equiv \begin{bmatrix} \pi_1 & ... & \pi_2 \end{bmatrix}^{\mathrm{T}}$ such that $\mathrm{A}\pi = 0$ where $\pi_n \neq 0$ for $n = 1, 2, 3, ..., N$ and $\sum_{n=1}^{N} \pi_n = 1$,

then

$$\begin{vmatrix} A_{22} & \cdots & A_{2N-1} & A_{2N} \\ \vdots & \ddots & \vdots & \vdots \\ A_{N-12} & \cdots & A_{N-1N-1} & A_{N-1N} \\ A_{N2} & \cdots & A_{NN-1} & A_{NN} \end{vmatrix} = \pi_1 \prod_{n=2}^{N} E_n \qquad 386$$

where E_n are the remaining eigenvalues for $n = 2, 3, 4, ..., N$, i.e., $\mathrm{AV}_n = E_n \mathrm{V}_n$ where V_n are the remaining eigenvectors.

To prove this statement, let us consider $\mathrm{A}(\varepsilon) \equiv \mathrm{A} + \varepsilon \mathrm{I}$ for $\varepsilon > 0$ which gives

$$\det(\mathrm{A}(\varepsilon)) = \begin{vmatrix} A_{11}+\varepsilon & A_{12} & \cdots & A_{1N-1} & A_{1N} \\ A_{21} & A_{22}+\varepsilon & \cdots & A_{2N-1} & A_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ A_{N-11} & A_{N-12} & \cdots & A_{N-1N-1}+\varepsilon & A_{N-1N} \\ A_{N1} & A_{N2} & \cdots & A_{NN-1} & A_{NN}+\varepsilon \end{vmatrix}. \qquad 387$$

From $\mathrm{A}(\varepsilon)\pi = \varepsilon\pi$ or $A_{i1}(\varepsilon) + \sum_{j=2}^{N} A_{ij}(\varepsilon)\frac{\pi_j}{\pi_1} = \varepsilon\frac{\pi_i}{\pi_1}$, equation (387) becomes

$$\det(\mathrm{A}(\varepsilon)) = \varepsilon \begin{vmatrix} 1 & A_{12} & \cdots & A_{1N-1} & A_{1N} \\ \frac{\pi_2}{\pi_1} & A_{22}+\varepsilon & \cdots & A_{2N-1} & A_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\pi_{N-1}}{\pi_1} & A_{N-12} & \cdots & A_{N-1N-1}+\varepsilon & A_{N-1N} \\ \frac{\pi_N}{\pi_1} & A_{N2} & \cdots & A_{NN-1} & A_{NN}+\varepsilon \end{vmatrix}. \qquad 388$$

Then, from $\sum_{i=1}^{N} A_{ij}(\varepsilon) = \varepsilon$ and $\sum_{n=1}^{N} \pi_n = 1$, equation (388) becomes

$$\det\left(\mathrm{A}\left(\varepsilon\right)\right)=\frac{\varepsilon}{\pi_1}\begin{vmatrix} 1 & \varepsilon & \cdots & \varepsilon & \varepsilon \\ \pi_2 & A_{22}+\varepsilon & \cdots & A_{2N-1} & A_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \pi_{N-1} & A_{N-12} & \cdots & A_{N-1N-1}+\varepsilon & A_{N-1N} \\ \pi_N & A_{N2} & \cdots & A_{NN-1} & A_{NN}+\varepsilon \end{vmatrix}. \tag{389}$$

Afterwards, we exploit the fact that $\det\left(\mathrm{A}\left(\varepsilon\right)\right)=\varepsilon\prod_{n=2}^{N}\left(E_n+\varepsilon\right)$, so

$$\begin{vmatrix} 1 & \varepsilon & \cdots & \varepsilon & \varepsilon \\ \pi_2 & A_{22}+\varepsilon & \cdots & A_{2N-1} & A_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \pi_{N-1} & A_{N-12} & \cdots & A_{N-1N-1}+\varepsilon & A_{N-1N} \\ \pi_N & A_{N2} & \cdots & A_{NN-1} & A_{NN}+\varepsilon \end{vmatrix}=\pi_1\prod_{n=2}^{N}\left(E_n+\varepsilon\right). \tag{390}$$

Finally, after taking limit $\varepsilon\to 0$ of this equation, we obtain

$$\begin{vmatrix} A_{22} & \cdots & A_{2N-1} & A_{2N} \\ \vdots & \ddots & \vdots & \vdots \\ A_{N-12} & \cdots & A_{N-1N-1} & A_{N-1N} \\ A_{N2} & \cdots & A_{NN-1} & A_{NN} \end{vmatrix}=\pi_1\prod_{n=2}^{N}E_n. \tag{391}$$

From this finding result, for a given irreducible and aperiodic Markov chain A, it can be shown that the vector $\boldsymbol{\pi}^*\equiv\begin{bmatrix}\pi_1^* & \cdots & \pi_N^*\end{bmatrix}^{\mathrm{T}}$, whose entries are defined as

$$\pi_i^*\equiv\frac{\left[\mathrm{adj}\left(\mathrm{I}-\mathrm{A}\right)\right]_{ij}}{\prod_{n=2}^{N}\left(1-E_n\right)} \tag{392}$$

for $i,j=1,2,3,\ldots,N$, is the eigenvector of A such that $\mathrm{A}\boldsymbol{\pi}^*=\boldsymbol{\pi}^*$ and $\sum_{n=1}^{N}\pi_n^*=1$. Note that $E_n\neq 1$ are the remaining eigenvalues of A, for $n=2,3,4,\ldots,N$.

The proof of the first condition, i.e., $\mathrm{A}\boldsymbol{\pi}^*=\boldsymbol{\pi}^*$

Plug π_i^* in equation (392) into the equation $\left[\mathrm{A}\boldsymbol{\pi}^*\right]_i=\sum_{j=1}^{N}A_{ij}\pi_j^*$,

$$\left[\mathrm{A}\boldsymbol{\pi}^*\right]_i=\sum_{j=1}^{N}A_{ij}\frac{\left[\mathrm{adj}\left(\mathrm{I}-\mathrm{A}\right)\right]_{jk}}{\prod_{n=2}^{N}\left(1-E_n\right)} \tag{393}$$

for any $k=1,2,3,\ldots,N$. Afterwards, use the definition of an adjugate matrix,

$$\left[\mathrm{A}\pi^*\right]_i = \frac{1}{\prod_{n=2}^{N}\left(1-E_n\right)}\sum_{j=1}^{N} A_{ij}\left(-1\right)^{k+j}\det\left(\mathrm{I}-\mathrm{A}\right)_{kj} \qquad 394$$

where $\det\left(\mathrm{I}-\mathrm{A}\right)_{kj}$ is defined as the determinant of the $\left(N-1\right)\times\left(N-1\right)$ matrix that results from deleting row k and column j of $\mathrm{I}-\mathrm{A}$. Now, let us add and subtract the term $\delta_{ij}\left(-1\right)^{k+j}\det\left(\mathrm{I}-\mathrm{A}\right)_{kj}$ in the sum,

$$\left[\mathrm{A}\pi^*\right]_i = \frac{-1}{\prod_{n=2}^{N}\left(1-E_n\right)}\sum_{j=1}^{N}\left(\delta_{ij}-A_{ij}-\delta_{ij}\right)\left(-1\right)^{k+j}\det\left(\mathrm{I}-\mathrm{A}\right)_{kj}, \qquad 395$$

and rearrange terms,

$$\left[\mathrm{A}\pi^*\right]_i = \frac{1}{\prod_{n=2}^{N}\left(1-E_n\right)}\left\{\left(-1\right)^{k+i}\det\left(\mathrm{I}-\mathrm{A}\right)_{ki} - \sum_{j=1}^{N}\left[\mathrm{I}-\mathrm{A}\right]_{ij}\left(-1\right)^{k+j}\det\left(\mathrm{I}-\mathrm{A}\right)_{kj}\right\}. \qquad 396$$

Finally, we employ the fact that the last term vanishes and obtain

$$\left[\mathrm{A}\pi^*\right]_i = \frac{\left[\mathrm{adj}\left(\mathrm{I}-\mathrm{A}\right)\right]_{ik}}{\prod_{n=2}^{N}\left(1-E_n\right)} = \pi_i^*. \qquad 397$$

The proof of the second condition, i.e., $\sum_{n=1}^{N}\pi_n^* = 1$

For any $j = 1,2,3,\ldots,N$, $\sum_{n=1}^{N}\pi_n^* = \sum_{i=1}^{N}\frac{\left[\mathrm{adj}\left(\mathrm{I}-\mathrm{A}\right)\right]_{ij}}{\prod_{n=2}^{N}\left(1-E_n\right)}$ or

$$\sum_{n=1}^{N}\pi_n^* = \frac{1}{\prod_{n=2}^{N}\left(1-E_n\right)}\sum_{i=1}^{N}\left(-1\right)^{j+i}\det\left(\mathrm{I}-\mathrm{A}\right)_{ji}. \qquad 398$$

Let us show $\sum_{i=1}^{N}\left(-1\right)^{j+i}\det\left(\mathrm{I}-\mathrm{A}\right)_{ji} = \sum_{i=1}^{N}\left(-1\right)^{1+i}\det\left(\mathrm{I}-\mathrm{A}\right)_{1i}$ for any $j = 1,2,3,\ldots,N$.

Let us begin with $j = 2$,

$$\sum_{i=1}^{N}\left(-1\right)^{2+i}\det\left(\mathrm{I}-\mathrm{A}\right)_{2i} = \begin{vmatrix} 1-A_{11} & -A_{12} & \cdots & -A_{1N-1} & -A_{1N} \\ 1 & 1 & \cdots & 1 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ -A_{N-11} & -A_{N-12} & \cdots & 1-A_{N-1N-1} & -A_{N-1N} \\ -A_{N1} & -A_{N2} & \cdots & -A_{NN-1} & 1-A_{NN} \end{vmatrix}. \qquad 399$$

$$\sum_{i=1}^{N}(-1)^{2+i}\det(\mathrm{I}-\mathrm{A})_{2i}=-\begin{vmatrix}1 & 1 & \cdots & 1 & 1\\ 1-A_{11} & -A_{12} & \cdots & -A_{1N-1} & -A_{1N}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ -A_{N-11} & -A_{N-12} & \cdots & 1-A_{N-1N-1} & -A_{N-1N}\\ -A_{N1} & -A_{N2} & \cdots & -A_{NN-1} & 1-A_{NN}\end{vmatrix}. \qquad 400$$

From $\sum_{i=1}^{N}\mathrm{A}_{ij}=1$ for any $j=1,2,3,...,N$,

$$\sum_{i=1}^{N}(-1)^{2+i}\det(\mathrm{I}-\mathrm{A})_{2i}=-\begin{vmatrix}1 & 1 & \cdots & 1 & 1\\ A_{21} & -(1-A_{22}) & \cdots & A_{2N-1} & A_{2N}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ -A_{N-11} & -A_{N-12} & \cdots & 1-A_{N-1N-1} & -A_{N-1N}\\ -A_{N1} & -A_{N2} & \cdots & -A_{NN-1} & 1-A_{NN}\end{vmatrix} \qquad 401$$

or $$\sum_{i=1}^{N}(-1)^{2+i}\det(\mathrm{I}-\mathrm{A})_{2i}=\sum_{i=1}^{N}(-1)^{1+i}\det(\mathrm{I}-\mathrm{A})_{1i}. \qquad 402$$

Analogously, it can be shown that this is true for the remaining $j=3,4,5,...,N$. Now let us consider

$$\sum_{i=1}^{N}(-1)^{1+i}\det(\mathrm{I}-\mathrm{A})_{1i}=\begin{vmatrix}1 & 1 & \cdots & 1 & 1\\ -A_{21} & 1-A_{22} & \cdots & -A_{2N-1} & -A_{2N}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ -A_{N-11} & -A_{N-12} & \cdots & 1-A_{N-1N-1} & -A_{N-1N}\\ -A_{N1} & -A_{N2} & \cdots & -A_{NN-1} & 1-A_{NN}\end{vmatrix}. \qquad 403$$

From the existence of π such that $\mathrm{A}\pi=\pi$ and $\sum_{n=1}^{N}\pi_n=1$ so

$$\sum_{i=1}^{N}(-1)^{1+i}\det(\mathrm{I}-\mathrm{A})_{1i}=\frac{1}{\pi_1}\begin{vmatrix}1-A_{22} & \cdots & -A_{2N-1} & -A_{2N}\\ \vdots & \ddots & \vdots & \vdots\\ -A_{N-12} & \cdots & 1-A_{N-1N-1} & -A_{N-1N}\\ -A_{N2} & \cdots & -A_{NN-1} & 1-A_{NN}\end{vmatrix}. \qquad 404$$

Since the matrix $\mathrm{I}-\mathrm{A}$ satisfies the conditions in the preceding discussion, from equation (391), equation (404) becomes

$$\sum_{i=1}^{N}(-1)^{1+i}\det(\mathrm{I}-\mathrm{A})_{1i}=\prod_{n=2}^{N}(1-E_n). \qquad 405$$

From equations (398), (402) and (405), we can conclude that

$$\sum_{n=1}^{N}\pi_n^{*}=1. \qquad 406$$

Appendix 5

From equation (111), we have

$$\langle x\rangle^{*}(s)=\frac{1}{i}\frac{\partial}{\partial k}\sum_{a=1}^{N}e^{ik\hat{x}\bullet\vec{r}_a}\tilde{\wp}^{*}\left(k,\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)\Big|_{k=0}. \tag{407}$$

After using the definition of the Fourier transform, we obtain

$$\langle x\rangle^{*}(s)=\frac{1}{i}\frac{\partial}{\partial k}\sum_{a=1}^{N}\sum_{m=-\infty}^{\infty}e^{ik\hat{x}\bullet\left(mL\hat{x}+\vec{r}_a\right)}\wp^{*}\left(mL\hat{x}+\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)\Big|_{k=0}. \tag{408}$$

Finally, after calculating the derivative, we obtain

$$\langle x\rangle^{*}(s)=\sum_{a=1}^{N}\sum_{m=-\infty}^{\infty}x_{m,a}\wp^{*}\left(\vec{x}_{m,a},s\,|\,\vec{x}_{0,b}\right). \tag{409}$$

It is analogous for the Laplace transform $\langle x^2\rangle^{*}(s)$ of the second moment.

Appendix 6

Consider the sum $\sum_{a=1}^{N}\tilde{\wp}^{*}\left(0,\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)$ of the Fourier-Laplace transform of $\wp\left(\vec{x}_{m,a},t\,|\,\vec{x}_{0,b}\right)$ at the point $k=0$, which can be calculated from

$$\sum_{a=1}^{N}\tilde{\wp}^{*}\left(0,\vec{r}_a,s\,|\,\vec{x}_{0,b}\right)=\int_{0}^{\infty}\left(\sum_{m=-\infty}^{\infty}\sum_{a=1}^{N}\wp\left(\vec{x}_{m,a},t\,|\,\vec{x}_{0,b}\right)\right)e^{-st}dt. \tag{410}$$

From the fact that a walker must be somewhere on the underlying structure at any time, i.e., $\sum_{m=-\infty}^{\infty}\sum_{a=1}^{N}\wp\left(\vec{x}_{m,a},t\,|\,\vec{x}_{0,b}\right)=1$, the right side of this equation is equal to $1/s$. On the other hand, the left side can be calculated from equations (86) and (87),

$$\frac{1-\psi^{*}(s)}{s}\sum_{a=1}^{N}\left\{\delta_{a,b}+\sum_{c=1}^{N_M}\bar{p}\left(0,\vec{r}_a,\vec{r}_c;\psi^{*}(s)\right)\frac{\mathrm{adj}\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(0;\psi^{*}(s)\right)\right]_{cb}}{\prod_{n=1}^{N_M}\left(1-E_n\left(0;\psi^{*}(s)\right)\right)}\right\}. \tag{411}$$

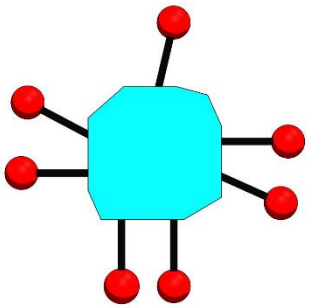
After combining everything together and using equations (81) and (85), we have

$$\frac{1-E_1\left(0;\psi^{*}(s)\right)}{1-\psi^{*}(s)}=\sum_{c=1}^{N_M}\left\{1+\sum_{a=N_M+1}^{N}\bar{p}\left(0,\vec{r}_a,\vec{r}_c;\psi^{*}(s)\right)\right\}\frac{\mathrm{adj}\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(0;\psi^{*}(s)\right)\right]_{cb}}{\prod_{n=2}^{N_M}\left(1-E_n\left(0;\psi^{*}(s)\right)\right)}. \tag{412}$$

For the diffusive random walks, i.e., $\sum_{a=1}^{N_M}\bar{p}\left(0,\vec{r}_a,\vec{r}_c;1^{-}\right)=1$, as $s\to 0^{+}$ we have

$$\frac{1-E_1\left(0;\psi^{*}(s)\right)}{1-\psi^{*}(s)}\sim\sum_{c=1}^{N_M}\sum_{a=1}^{N}\bar{p}\left(0,\vec{r}_a,\vec{r}_c;\psi^{*}(s)\right)\frac{\mathrm{adj}\left[\mathrm{I}\text{-}\bar{\mathrm{p}}\left(0;\psi^{*}(s)\right)\right]_{cb}}{\prod_{n=2}^{N_M}\left(1-E_n\left(0;\psi^{*}(s)\right)\right)}. \tag{413}$$

Appendix 7



A schematic of a network lattice with seven different absorbing sites.

Let us consider a network lattice with N different absorbing sites. A schematic of such structure is shown in the above figure where red spheres are represented the absorbing sites labelled by $a = 1, 2, 3, ..., N$. The probability of being absorbed at step n th, given that the walker initially commenced from the absorbing site a, is denoted by $u_{a,n}$. For the complimentary event, the walker is not absorbed at the n th, the probability is denoted by $f_{a,n} \equiv 1 - \sum_{i=0}^{n} u_{a,i}$. In addition, if the walker is not absorbed at the n th, then the walker must be found at any site, which is not an absorbing site, at the n th step. In other words, if $p_{ba,n}$ is defined as the probability that the walker is found at a certain site b, which is not an absorbing site, at the n th step for $n > 0$, given that the walker initially commenced from the absorbing site a, then $f_{a,n} = \sum_{b} p_{ba,n}$ where the summation is over all possible site which is not an absorbing site.

From the preceding description, it is not hard to show that, for $-1 < \xi < 1$, the generating function $u_a(\xi) \equiv \sum_{n=0}^{\infty} u_{a,n} \xi^n$ has a simple relation to the generating function $f_a(\xi) \equiv \sum_{n=0}^{\infty} f_{a,n} \xi^n$, i.e.,

$$1 - u_a(\xi) = (1 - \xi) f_a(\xi) \qquad 414$$

which gives

$$1 - u_a(\xi) \sim (1 - \xi) \lim_{\xi \to 1^-} f_a(\xi) \qquad 415$$

if the limit $\lim_{\xi\to 1^-} f_a(\xi)$ exists.

If the walker is eventually absorbed, i.e., $\lim_{\xi\to 1^-} u_a(\xi) = \sum_{n=0}^{\infty} u_{n,a} = 1$ and the mean absorbing time τ_a is finite, i.e., $\tau_a \equiv \lim_{\xi\to 1^-} \frac{du_a(\xi)}{d\xi} = \sum_{n=0}^{\infty} n u_{n,a} < \infty$, then, after finding the limit $\xi \to 1^-$ of the derivative of equation (414) with respect to ξ, we obtain

$$\lim_{\xi\to 1^-} f_a(\xi) = \tau_a . \qquad 416$$

Additionally, as $f_{a,0} = 1$ and $\sum_{\vec{r}} p(\vec{r} \mid \vec{r}_a)_0 = 0$, the mean absorbing time can also be calculated from $\tau_a = 1 + \sum_{n=0}^{\infty}\sum_{b} p_{ba,n}$ or

$$\tau_a = 1 + \lim_{\xi\to 1^-} \sum_{b} p_{ba}(\xi) . \qquad 417$$

This result can be generalized to the case that the initially commencing sites are not regraded. In this case, the probability u_n of being absorbed at step nth is defined as $u_n \equiv \sum_{a=1}^{N} u_{a,n}\pi_a$ where π_a is the probability that the walker initially commenced from the absorbing site a. From the linearity, the previous analysis can also be applied to the probability u_n, and the result is

$$1 - u(\xi) \sim (1-\xi)G \qquad 418$$

where the mean number of steps G before absorption can be calculate from

$$G = \lim_{\xi\to 1^-} \frac{du(\xi)}{d\xi} \qquad 419$$

or

$$G = \sum_{a=1}^{N}\left(1 + \lim_{\xi\to 1^-} \sum_{b} p_{ba}(\xi)\right)\pi_a \qquad 420$$

Therefore, when the eigenfunction $E_1(0;\xi)$ satisfies the conditions of the generating function $u(\xi)$, the resulting equation (418) – (420) can also be employed.

Appendix 8

Let us consider the contour integral

$$f(m;\xi)=-\frac{1}{\alpha^*(\xi)}\times\frac{1}{2\pi i}\oint_{\mathcal{C}}\frac{z^{-m}}{\left(z^2-\left(\frac{1}{\alpha^*(\xi)}-\frac{\Sigma(\xi)}{\alpha^*(\xi)}\right)z-\frac{\gamma^*(\xi)}{\alpha^*(\xi)}\right)}dz. \qquad 421$$

As $\Phi(\xi)\equiv 1-\Sigma(\xi)$, $\Gamma(\xi)\equiv\sqrt{\Phi^2(\xi)-4\alpha^*(\xi)\gamma^*(\xi)}$ and $A_{\pm}(\xi)\equiv\frac{1}{2\alpha^*(\xi)}\left(\Phi(\xi)\pm\Gamma(\xi)\right)$, this equation becomes

$$f(m;\xi)=-\frac{1}{\alpha^*(\xi)}\times\frac{1}{2\pi i}\oint_{\mathcal{C}}\frac{z^{-m}}{\left(z-A_+(\xi)\right)\left(z-A_-(\xi)\right)}dz. \qquad 422$$

All scenarios we consider satisfy the conditions that, for $-1<\xi<1$, $0<A_-(\xi)<1$ and $1<A_+(\xi)$ which implies that the singularity $A_-(\xi)$ is in a region bounded by the unit circle $\mathcal{C}$, while the singularity $A_+(\xi)$ is outside this region. From the residue theorem, the result for $m\le 0$ is straight forward because there is only one simple pole in the region,

$$f(m;\xi)=\frac{1}{\Gamma(\xi)}\left(\frac{\left(\Phi(\xi)-\Gamma(\xi)\right)}{2\alpha^*(\xi)}\right)^{|m|}. \qquad 423$$

The result of the integral for $m>0$ is identical to the result of the integral for $m<0$ with interchanging the function $\alpha^*(\xi)$ and the function $\gamma^*(\xi)$. Altogether, we have

$$f(m;\xi)=\frac{1}{\Gamma(\xi)}\left(\frac{1}{2}\left(\Phi(\xi)-\Gamma(\xi)\right)\right)^{|m|}\times\begin{cases}\left(\gamma^*(\xi)\right)^{-|m|} & ;m>0\\ \left(\alpha^*(\xi)\right)^{-|m|} & ;m\le 0\end{cases}. \qquad 424$$

The integral

$$P_{11}(m;\xi)=-\frac{1}{\alpha\xi}\times\frac{1}{2\pi i}\oint_{\mathcal{C}}\left(z^2-\left(\frac{1}{\alpha\xi}-\frac{\beta}{\alpha\xi}\right)z-\frac{\gamma}{\alpha}\right)^{-1}z^{-m}dz \qquad 425$$

is the special case of the preceding integral for $\alpha^*(\xi)=\alpha\xi$, $\gamma^*(\xi)=\gamma\xi$ and $\Sigma^*(\xi)=\beta\xi$.

Appendix 9

The derivation for $p_1^{(H)} \equiv \left(1+\left(\frac{\gamma}{\alpha}\right)^{1/(1-N)}\right)^{-1}$

From $\vartheta = \frac{\left(\alpha^* - \gamma^*\right)N}{\Gamma(1+v)Gt_0^v}$, let us consider $\alpha^* - \gamma^*$.

$$\alpha^* - \gamma^* = \alpha\left(\frac{\lambda_+(p)-\lambda_-(p)}{\left(\lambda_+(p)\right)^N+\left(\lambda_-(p)\right)^N}\right)-\gamma\left(\frac{\lambda_+(q)-\lambda_-(q)}{\left(\lambda_+(q)\right)^N+\left(\lambda_-(q)\right)^N}\right).$$

$$\alpha^* - \gamma^* = \gamma\left(\frac{\lambda_+(q)-\lambda_-(q)}{\left(\lambda_+(q)\right)^N+\left(\lambda_-(q)\right)^N}\right) \times\left\{\frac{\alpha}{\gamma}\left(\frac{\lambda_+(p)-\lambda_-(p)}{\left(\lambda_+(p)\right)^N+\left(\lambda_-(p)\right)^N}\right)\left(\frac{\left(\lambda_+(q)\right)^N+\left(\lambda_-(q)\right)^N}{\lambda_+(q)-\lambda_-(q)}\right)-1\right\}.$$

$$\alpha^* - \gamma^* = \gamma\left(\frac{\lambda_+(q)-\lambda_-(q)}{\left(\lambda_+(q)\right)^N+\left(\lambda_-(q)\right)^N}\right)\left(\frac{\alpha}{\gamma}\left(\frac{p}{q}\right)^{N-1}-1\right);\ \lambda_\pm(q)=\frac{p}{q}\lambda_\pm(p).$$

$$\alpha^* - \gamma^* = \gamma\left(\frac{\lambda_+(q)-\lambda_-(q)}{\left(\lambda_+(q)\right)^N+\left(\lambda_-(q)\right)^N}\right)\left(\frac{\alpha}{\gamma}\left(\frac{1}{1/p-1}\right)^{N-1}-1\right);\ p+q=1.$$

$$\alpha^* - \gamma^* = \gamma\left(\frac{\lambda_+(q)-\lambda_-(q)}{\left(\lambda_+(q)\right)^N+\left(\lambda_-(q)\right)^N}\right)\left(\left(\frac{(\gamma/\alpha)^{1/(1-N)}}{1/p-1}\right)^{N-1}-1\right).$$

$$\alpha^* - \gamma^* = \gamma\left(\frac{\lambda_+(q)-\lambda_-(q)}{\left(\lambda_+(q)\right)^N+\left(\lambda_-(q)\right)^N}\right)\left(\left(\frac{\left((\gamma/\alpha)^{1/(1-N)}+1\right)-1}{1/p-1}\right)^{N-1}-1\right).$$

Therefore, if $1/p=(\gamma/\alpha)^{1/(1-N)}+1$ or

$$p = p_1^{(H)} \equiv \left(1+(\gamma/\alpha)^{1/(1-N)}\right)^{-1},$$

then $\alpha^* - \gamma^* = 0$ and $\vartheta = 0$.

Appendix 10

The derivation for $p_2^{(H)} \equiv \frac{1}{2}\left(1+\frac{\alpha-\gamma}{1+\beta\tau_\beta}\right)$

From $\vartheta = c\frac{N}{\Gamma(1+v)t_0^v}$ where $c \equiv \frac{\left(\alpha^*-\gamma^*\right)}{\left(1+\alpha\tau_\alpha+\gamma\tau_\gamma+\beta\tau_\beta\right)}$,

$$c = \frac{\left(\alpha-\gamma a^{N-1}\right)\left(\frac{1-a}{1-a^N}\right)}{\left(1+\beta\tau_\beta\right)+\frac{\alpha}{q-p}\left(1-N\left(\frac{1-a}{1-a^N}\right)\right)+\frac{\gamma}{q-p}\left(\left(N-1\right)-N\left(\frac{1-a^{N-1}}{1-a^N}\right)\right)}.$$

$$c = \frac{(2p-1)\left(\alpha-\gamma a^{N-1}\right)\left(\frac{1-a}{1-a^N}\right)}{\left((2p-1)\left(1+\beta\tau_\beta\right)-\alpha\left(1-N\left(\frac{1-a}{1-a^N}\right)\right)-\gamma\left(\left(N-1\right)-N\left(\frac{1-a^{N-1}}{1-a^N}\right)\right)\right)};\ p+q=1.$$

$$c = \frac{(2p-1)\left(\alpha-\gamma a^{N-1}\right)\left(\frac{1-a}{1-a^N}\right)}{\left((2p-1)\left(1+\beta\tau_\beta\right)-\left(\alpha-\gamma\right)+\left(\alpha N\left(\frac{1-a}{1-a^N}\right)\right)+\gamma N\left(1-\frac{1-a^{N-1}}{1-a^N}\right)\right)}.$$

$$c = \frac{(2p-1)\left(\alpha-\gamma a^{N-1}\right)\left(\frac{1-a}{1-a^N}\right)}{\left((2p-1)\left(1+\beta\tau_\beta\right)-\left(\alpha-\gamma\right)+\left(\alpha N\left(\frac{1-a}{1-a^N}\right)\right)+\gamma a^{N-1}N\left(\frac{1-a}{1-a^N}\right)\right)}.$$

$$c = \frac{(2p-1)\left(\alpha-\gamma a^{N-1}\right)\left(\frac{1-a}{1-a^N}\right)}{(2p-1)\left(1+\beta\tau_\beta\right)-\left(\alpha-\gamma\right)+\left(\alpha-\gamma a^{N-1}\right)\left(\frac{1-a}{1-a^N}\right)N}.$$

Therefore, if $(2p-1)\left(1+\beta\tau_\beta\right)=\left(\alpha-\gamma\right)$ or

$$p = p_2^{(H)} \equiv \frac{1}{2}\left(1+\frac{\alpha-\gamma}{1+\beta\tau_\beta}\right),$$

then $\vartheta = \frac{(2p_2^{(H)}-1)}{\Gamma(1+v)t_0^v} = \frac{\alpha-\gamma}{1+\beta\tau_\beta}\left(\frac{1}{\Gamma(1+v)t_0^v}\right)$.

Appendix 11

The derivation for $p_3^{(H)} = \left(1+\frac{\gamma}{\alpha}\right)^{-1}$

$$\alpha^* - \gamma^* = \left(\alpha - \gamma a^{N-1}\right)\left(\frac{1-a}{1-a^N}\right).$$

$$\alpha^* - \gamma^* = \alpha\left(1-\frac{\gamma}{\alpha}a^{N-1}\right)\left(\frac{1-a}{1-a^N}\right).$$

$$\alpha^* - \gamma^* = \frac{\left(1-\frac{\gamma}{a\alpha}a^N\right)}{1-a^N}\left(\alpha - a\alpha\right).$$

$$\alpha^* - \gamma^* = \frac{\left(1-\frac{\gamma}{\left(\frac{1-p}{p}\right)\alpha}a^N\right)}{1-a^N}\left(\alpha - \left(\frac{1-p}{p}\right)\alpha\right) \; ; a \equiv q/p \, .$$

$$\alpha^* - \gamma^* = \frac{\left(1-\frac{\left(1+\gamma/\alpha\right)-1}{1/p-1}a^N\right)}{1-a^N}\left(\alpha - \gamma\left(\frac{1/p-1}{\left(1+\gamma/\alpha\right)-1}\right)\right).$$

Therefore, if $1/p = 1+\gamma/\alpha$ or

$$p = p_3^{(H)} \equiv \left(1+\frac{\gamma}{\alpha}\right)^{-1},$$

then $\alpha^* - \gamma^* = \alpha - \gamma$.

Appendix 12

Let $-1<\xi<1$, $m\le 0$, $|A_{+-}(\xi)|,|A_{--}(\xi)|<1$, $1<|A_{++}(\xi)|,|A_{+-}(\xi)|$ and the function $H(z)$ be a non-singularity function. From the residue theorem, it can be shown that

$$f(m;\xi)=\frac{1}{2\pi i}\oint_{\mathcal{C}}\frac{H(z)z^{-m}}{\left(z-A_{++}(\xi)\right)\left(z-A_{+-}(\xi)\right)\left(z-A_{-+}(\xi)\right)\left(z-A_{--}(\xi)\right)}dz, \tag{426}$$

where the contour $\mathcal{C}$ is the unit circle, is equal to

$$\begin{aligned} f(m;\xi) \quad =&\frac{H\left(A_{+-}(\xi)\right)\left(A_{+-}(\xi)\right)^{|m|}}{\left(A_{+-}(\xi)-A_{++}(\xi)\right)\left(A_{+-}(\xi)-A_{-+}(\xi)\right)\left(A_{+-}(\xi)-A_{--}(\xi)\right)}+\\ &\frac{H\left(A_{--}(\xi)\right)\left(A_{--}(\xi)\right)^{|m|}}{\left(A_{--}(\xi)-A_{++}(\xi)\right)\left(A_{--}(\xi)-A_{-+}(\xi)\right)\left(A_{--}(\xi)-A_{+-}(\xi)\right)}. \end{aligned} \tag{427}$$

Appendix 13

The aim of this appendix is to factorize the function

$$\prod_{a=\pm}\left(1-\left(\alpha_a^*(\xi)\left(z+z^{-1}\right)+\Sigma_a(\xi)\right)\right)-\prod_{a=\pm}\beta_a^*(\xi)\cdot \tag{428}$$

First, let us substitute the term $z+z^{-1}$ by $2Z$,

$$\left(1-\left(2\alpha_+^*(\xi)Z+\Sigma_+(\xi)\right)\right)\left(1-\left(2\alpha_-^*(\xi)Z+\Sigma_-(\xi)\right)\right)-\beta_+^*(\xi)\beta_-^*(\xi)\cdot \tag{429}$$

Then assume that $\alpha_\pm^*(\xi)\neq 0$ and rewritten this expression as

$$4\alpha_-^*(\xi)\alpha_+^*(\xi)\left(\left(Z-\frac{1-\Sigma_+(\xi)}{2\alpha_+^*(\xi)}\right)\left(Z-\frac{1-\Sigma_-(\xi)}{2\alpha_-^*(\xi)}\right)-\frac{\beta_+^*(\xi)\beta_-^*(\xi)}{4\alpha_-^*(\xi)\alpha_+^*(\xi)}\right). \tag{430}$$

After rewriting this in the form of a quadratic function of Z, it can be factorized,

$$4\alpha_-^*(\xi)\alpha_+^*(\xi)\left(Z-B_1(\xi)\right)\left(Z-B_2(\xi)\right), \tag{431}$$

where $B_{1,2}(\xi)\equiv\dfrac{\alpha_-^*(\xi)\left(1-\Sigma_+(\xi)\right)+\alpha_+^*(\xi)\left(1-\Sigma_-(\xi)\right)\pm K(\xi)}{4\alpha_+^*(\xi)\alpha_-^*(\xi)}$, 432

$$K(\xi)\equiv\sqrt{\left(2\alpha_-^*(1-\Sigma_+)+2\alpha_+^*(1-\Sigma_-)\right)^2-16\alpha_+^*\alpha_-^*\left((1-\Sigma_+)(1-\Sigma_-)-\beta_-^*\beta_+^*\right)}. \tag{433}$$

Afterwards, replace Z by $\left(z+z^{-1}\right)/2$, we have

$$\alpha_-^*(\xi)\alpha_+^*(\xi)\left(z+z^{-1}-2B_1(\xi)\right)\left(z+z^{-1}-2B_2(\xi)\right)\cdot \tag{434}$$

As terms in parentheses are quadratic functions of z, they are easy to be factorized,

$$\frac{\alpha_-^*(\xi)\alpha_+^*(\xi)}{z^2}\left(z-z^{(1)}(\xi)\right)\left(z-z^{(2)}(\xi)\right)\left(z-A^{(1)}(\xi)\right)\left(z-A^{(2)}(\xi)\right) \tag{435}$$

where $z^{(a)}(\xi)=B_a(\xi)-\sqrt{B_a^2(\xi)-1}$ and $A^{(a)}(\xi)=B_a(\xi)+\sqrt{B_a^2(\xi)-1}$ for $a=1,2$.

Appendix 14

For $N \geq 3$, it can be shown that the determinate of the $N \times N$ matrix

$$\mathrm{p}_N \equiv \begin{bmatrix} a & b & \cdots & 0 & b \\ b & a & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & a & b \\ b & 0 & \cdots & b & a \end{bmatrix} \tag{436}$$

is equal to

$$\det\left[\mathrm{p}_N\right] = a\left(\det\left[\mathrm{T}_{N-1}\right]\right) - 2b\left(b\left(\det\left[\mathrm{T}_{N-2}\right]\right) + (-1)^N b^{N-1}\right) \tag{437}$$

where T_{N-1} is the $(N-1)\times(N-1)$ matrix that results from deleting the first row and the first column of p_N.

To see this, let us consider the determinates of the matrices p_3 and p_4. For the matrix

$$\mathrm{p}_3 \equiv \begin{bmatrix} a & b & b \\ b & a & b \\ b & b & a \end{bmatrix}, \tag{438}$$

we have

$$\det\left[\mathrm{p}_3\right] = a\begin{vmatrix} a & b \\ b & a \end{vmatrix} - b\begin{vmatrix} b & b \\ b & a \end{vmatrix} + b\begin{vmatrix} b & b \\ a & b \end{vmatrix}. \tag{439}$$

As you may notice, the second and the third terms are identical,

$$\det\left[\mathrm{p}_3\right] = a\begin{vmatrix} a & b \\ b & a \end{vmatrix} - 2b\begin{vmatrix} b & b \\ b & a \end{vmatrix}, \tag{440}$$

and this determinate can be rewritten as

$$\det\left[\mathrm{p}_3\right] = a\left(\det\left[\mathrm{T}_2\right]\right) - 2b\left(b\left(\det\left[\mathrm{T}_1\right]\right) - b^2\right). \tag{441}$$

we have defined $\mathrm{T}_1 \equiv [a]$ and $\mathrm{T}_2 \equiv \begin{bmatrix} a & b \\ b & a \end{bmatrix}$ for notation consistency. Then, for the matrix

$$\mathrm{p}_4 \equiv \begin{bmatrix} a & b & 0 & b \\ b & a & b & 0 \\ 0 & b & a & b \\ b & 0 & b & a \end{bmatrix}, \tag{442}$$

we have

$$\det\left[\mathrm{p}_4\right]=a\begin{vmatrix}a & b & 0\\ b & a & b\\ 0 & b & a\end{vmatrix}-b\begin{vmatrix}b & 0 & b\\ b & a & b\\ 0 & b & a\end{vmatrix}-b\begin{vmatrix}b & 0 & b\\ a & b & 0\\ b & a & b\end{vmatrix}. \tag{443}$$

Again, the second and the third terms are identical,

$$\det\left[\mathrm{p}_4\right]=a\begin{vmatrix}a & b & 0\\ b & a & b\\ 0 & b & a\end{vmatrix}-2b\begin{vmatrix}b & 0 & b\\ b & a & b\\ 0 & b & a\end{vmatrix}, \tag{444}$$

and this determinate can be rewritten as

$$\det\left[\mathrm{p}_4\right]=a\left(\det\left[\mathrm{T}_3\right]\right)-2b\left(b\left(\det\left[\mathrm{T}_2\right]\right)+b^3\right) \tag{445}$$

where $T_3\equiv\begin{bmatrix}a & b & 0\\ b & a & b\\ 0 & b & a\end{bmatrix}$. Accordingly, the determination of the determinate of the matrix

$$\mathrm{p}_N\equiv\begin{bmatrix}a & b & \cdots & 0 & b\\ b & a & \cdots & 0 & 0\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & \cdots & a & b\\ b & 0 & \cdots & b & a\end{bmatrix} \tag{446}$$

is analogous to that of the matrix p_4, and we have

$$\det\left[\mathrm{p}_N\right]=a\left(\det\left[\mathrm{T}_{N-1}\right]\right)-2b\left(b\left(\det\left[\mathrm{T}_{N-2}\right]\right)+\left(-1\right)^N b^{N-1}\right). \tag{447}$$

Moreover, we notice that $\det\left[\mathrm{T}_N\right]$ satisfies the recurrence relation

$$\det\left[\mathrm{T}_N\right]=a\det\left[\mathrm{T}_{N-1}\right]-b^2\det\left[\mathrm{T}_{N-2}\right], \tag{448}$$

for $N=1,2,3,\ldots$ where $\det\left[\mathrm{T}_{-1}\right]=0$ and $\det\left[\mathrm{T}_0\right]=1$, and we can solve this linear difference equation with the generating function technique. For $N\geq 0$, we find

$$\det\left[\mathrm{T}_N\right]=U_N\left(\frac{a}{2b}\right)b^N \tag{449}$$

where $U_N\left(x\right)$ is the Chebyshev polynomial of the second kind for $-1\leq x\leq 1$. Therefore, equation (447) becomes

$$\det\left[\mathrm{p}_N\right]=2b^N\left(\frac{a}{2b}U_{N-1}\left(\frac{a}{2b}\right)-U_{N-2}\left(\frac{a}{2b}\right)-\left(-1\right)^N\right). \tag{450}$$

We can factorize the term on the right-hand side of this equation by finding the roots of the following equation

$$xU_{N-1}(x)-U_{N-2}(x)-1=0 \tag{451}$$

where $x\equiv\frac{a}{-2b}$. By employing one of the representations of the Chebyshev polynomials of the second kind,

$$U_N\left(\cos(\theta)\right)=\frac{\sin\left((N+1)\theta\right)}{\sin(\theta)}, \tag{452}$$

we find that the roots are

$$x_i=\cos\left(\frac{2\pi i}{N}\right) \tag{453}$$

for $i=0,1,2,...,N-1$. Consequently, equation (450) becomes

$$\det\left[\mathrm{p}_N\right]=(2b)^N\prod_{i=1}^{N}\left(\frac{a}{-2b}-\cos\left(\frac{2\pi(i-1)}{N}\right)\right) \tag{454}$$

or

$$\det\left[\mathrm{p}_N\right]=\prod_{i=1}^{N}\left(a-2\cos\left(\frac{2\pi(i-1)}{N}\right)(-b)\right) \tag{455}$$

for $-1\le\frac{a}{-2b}\le 1$.

Appendix 15

To determine the first term of the generating function

$$P_{ab}(m;\xi)=\sum_{i=1}^{N_M}\left(z^{(i)}(\xi)\right)^{|m|}P_{ab}^{(i)}(\xi) \tag{456}$$

for the matrix $\bar{\mathrm{p}}\left(k(z);\xi\right)$ satisfying equations (341) and (344), let us begin with rewriting the determinate $\det\left[\mathrm{I}-\bar{\mathrm{p}}\left(k(z);\xi\right)\right]$ in appropriate form. Using equation (455), we have

$$\begin{aligned}&\det\left[\mathrm{I}-\bar{\mathrm{p}}\left(k(z);\xi\right)\right]\\&=\left(1-\left(\alpha^*(\xi)\left(z^{-1}+z\right)+\Sigma(\xi)+2\beta^*(\xi)\right)\right)\prod_{i=2}^{N_M}\left(1-E_i(z;\xi)\right)\end{aligned} \tag{457}$$

where $E_i(z;\xi)=\bar{p}_{11}\left(k(z);\xi\right)+2\cos\left(\frac{2\pi(i-1)}{N_M}\right)\bar{p}_{21}\left(k(z);\xi\right)$. The first term on the right-hand side of equation (457) can be easily factorized,

$$\det\left[\mathrm{I}-\bar{\mathrm{p}}\left(k(z);\xi\right)\right]=\frac{\alpha^*(\xi)}{z}\left(z-z^{(1)}(\xi)\right)\left(z-A^{(1)}(\xi)\right)\prod_{i=2}^{N_M}\left(1-E_i(z;\xi)\right) \tag{458}$$

where

$$z^{(1)}(\xi)=\frac{1}{2\alpha^{*}(\xi)}\left(\left(1-\Sigma(\xi)-2\beta^{*}(\xi)\right)-\sqrt{\left(1-\Sigma(\xi)-2\beta^{*}(\xi)\right)^{2}-\left(2\alpha^{*}(\xi)\right)^{2}}\right) \quad 459$$

and $$A^{(1)}(\xi)=\frac{1}{2\alpha^{*}(\xi)}\left(\left(1-\Sigma(\xi)-2\beta^{*}(\xi)\right)+\sqrt{\left(1-\Sigma(\xi)-2\beta^{*}(\xi)\right)^{2}-\left(2\alpha^{*}(\xi)\right)^{2}}\right).$$

To determine the term $P_{ab}^{(1)}(\xi)$, we now consider the integral

$$P_{ab}(m;\xi)=\frac{1}{2\pi i\alpha^{*}(\xi)}\oint_{C}\frac{\mathrm{adj}\left[\mathrm{I}-\bar{\mathrm{p}}\left(k(z);\xi\right)\right]_{ab}}{\left(z-z^{(1)}(\xi)\right)\left(z-A^{(1)}(\xi)\right)\prod_{i=2}^{N_M}\left(1-E_i(z;\xi)\right)}z^{-m}dz. \quad 460$$

From the residue theorem, we obtain

$$P_{ab}(m;\xi) = \frac{1}{\alpha^{*}(\xi)\left(z^{(1)}(\xi)-A^{(1)}(\xi)\right)}\frac{\mathrm{adj}\left[\mathrm{I}-\bar{\mathrm{p}}\left(k\left(z^{(1)}\right);\xi\right)\right]_{ab}}{\prod_{i=2}^{N_M}\left(1-E_i\left(z^{(1)};\xi\right)\right)}\left(z^{(1)}(\xi)\right)^{|m|} + \sum_{i=2}^{N_M}\left(z^{(i)}(\xi)\right)^{|m|}P_{ab}^{(i)}(\xi) \quad 461$$

and

$$P_{ab}^{(1)}(\xi)=\frac{\mathrm{adj}\left[\mathrm{I}-\bar{\mathrm{p}}\left(k\left(z^{(1)}(\xi)\right);\xi\right)\right]_{ab}\Big/\prod_{i=2}^{N_M}\left(1-E_i\left(z^{(1)}(\xi);\xi\right)\right)}{\sqrt{\left(1-\Sigma(\xi)-2\beta^{*}(\xi)\right)^{2}-\left(2\alpha^{*}(\xi)\right)^{2}}}. \quad 462$$

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