Mathematical Analysis of k-path Laplacian Operators on Simple Graphs

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This thesis is the result of the author's original research. It has been composed by the author and has not been previously submitted for examination which has led to the award of a degree.

Name:

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Abstract

A set of links and nodes are the fundamental units or components used to represent complex networks. Over the last few decades, network studies have expanded and matured, increasingly making use of complex mathematical tools. Complex networks play a significant role in the propagation of processes, which include for example the case of epidemic spreading, the diffusion process, synchronisation or the consensus process. Such dynamic processes are critically important in achieving understanding of the behaviour of complex systems at different levels of complexity – examples might be the brain and modern man-made infrastructures. Although part of the study of the diffusion of information in the dynamic processes, it is generally supposed that interactions in networks originate only from a node, spreading to its nearest neighbours, there also exist long-range interactions (LRI), which can be transmitted from a node to others not directly connected.

The focus of this study is on dynamic processes on networks where nodes interact with not only their nearest neighbours but also through certain LRIs. The generalised $k-$path Laplacian operators (LOs) L_k, which account for the hop of a diffusive particle to its non-nearest neighbours in a graph, control this diffusive process, describing hops of nodes v_i at distance k; here the distance is measured as the length of the shortest path between two nodes. In this way the introduction of the k-path LOs can facilitate conducting more precise studies of network dynamics in different applications. This thesis aims to study a gener-

alised diffusion equation employing the transformed generalised k-path LOs for a locally finite infinite graph. This generalised diffusion equation promotes both normal and superdiffusive processes on infinite graphs.

Furthermore, this thesis develops a new theoretical mathematical framework for describing superdiffusion processes that use a transform of the k-path LOs defined on infinite graphs. The choice of the transform appeared to be vitally important as the probability of a long jump should be great enough. As described by other researchers the fractional diffusion equation (FDE) formed the mathematical framework employed to describe this anomalous diffusion. In this regard, it is taken that the diffusive particle is not just hopping to its nearest node but also to any other node of the network with a probability that scales according to the distance between the two places. Initially, we extend the k-path LOs above to consider a connected and locally finite infinite network with a bounded degree and investigate a number of the properties of these operators, such as their self-adjointness and boundedness. Then, three different transformations of the k-path LOs, i.e. the Laplace, Factorial and Mellin transformations as well as their properties, are studied.

In addition, in order to show a number of applications of these operators and the transformed ones, the transformed k-path LOs are used to obtain a generalised diffusion process for one-dimensional and two-dimensional infinite graphs. First, the infinite path graph is studied, where it is possible to prove that when the Laplacian- and factorial-transformed operators are used in the generalised diffusion equation, the diffusive processes observed are always normal, independent of the transform parameters. It is then proven analytically that when the k-path LOs are transformed via a Mellin transform and plugged into the diffusion equation, the result is a superdiffusive process for certain values of the exponent in the transform. Secondly, we generalise the results on the superdiffusive behaviour generated by transforming k-path LOs from one-dimensional graphs to

2-dimensional ones. Our attention focuses on the *Abstract Cauchy* problem in an infinite square lattice. A generalised diffusion equation on a square lattice corresponding to Mellin transforms of the k-path Laplacian is investigated. Similar to the one-dimensional case also for the graph embedded in two-dimensional space, we could observe superdiffusive behaviour for the Mellin transformed k-path Laplacian. In comparison to the one-dimensional case, the conclusion reached is that the asymptotic behaviour of the solution of the Cauchy problem is much subtler.

Publications and Presentations

The following papers were published in the course of the work contained in this thesis.

- E. Estrada, E. Hameed, N. Hatano, M. Langer: Path Laplacian operators and superdiffusive processes on graphs. I. One-dimensional case. *Linear Algebra Appi.* 523 (2017), 307–334.

- E. Estrada, E. Hameed, M. Langer, A. Puchalska: Path Laplacian operators and superdiffusive processes on graphs. II. Two-dimensional lattice. *Linear Algebra Appi.* 555 (2018), 373-397.

Some parts of this work have also been presented at the following

- E. Estrada, E. Hameed, N. Hatano, M. Langer: Mathematical analysis of k-path Laplacian operators on networks. Presented at the 1st edition of "Latin American Conference on Complex Networks" (LANET), Puebla, México, 2017.

- E. Estrada, E. Hameed, N. Hatano, M. Langer: Dynamical processes modelled by k-path Laplacian operators. Presented at the 6th International Conference on Complex Networks and their Applications, Lyon, France, 2017.

Contents

List of Figures

Introduction

0.1 Complex Systems

A concept that pervades our daily lives and changes the way we approach science, medicine, economics, business, and even the study of intelligence in natural and artificial systems is that of complexity. Complex system models can represent a range of real-life phenomena and reproduce, with a certain degree of success, situations such as cellular interactions, chemical reaction-diffusion systems, stock market dynamics, motorway traffic, neuronal interactions, or the way opinions are formed in social systems. Further examples, among many, include the flow of power grids, internet dynamics, airline transportation, and street plans. Complex systems are systems that comprise a multitude of interconnected parts able to interact and generate a new quality of collective behaviour by means of self-organisation, i.e., the spontaneous formation of temporal, spatial or functional structures [28]. Complex systems are not simply their parts totalled up. Among the characteristics often attributed to them are extreme sensitivity to initial conditions as well as emergent behaviours that are not readily predictable or even completely deterministic [81]. Network Science has become a significant framework to model, analyse, simulate and design such complex systems. The definition of a network could be that it is a diagrammatic representation of a system comprising nodes or vertices, representing the entities of the system. Links or edges join these nodes, representing a certain kind of interconnection among them [36].

Networks are graphs that represent or model observable reality. An important concept in this field is: the structure and attributes of the network influence its dynamical properties.

The network is the main skeleton of complex systems, and ubiquitous in natural and man-made environments, which range from the social and ecological to the biology and infrastructure [36, 86, 87, 88]. The revelation of the essential qualities of the networks was aided by fortuity, inventiveness and experimental collection of data. Networks have been used extensively in the social sciences to represent interpersonal relationships [4]. In such cases, the vertices correspond to individuals in a group or society, and the edges join pairs of individuals who are related in some way. For example, there is a link between individuals x and y if x likes, hates, agrees with, avoids, or communicates with individual y. Such representations are extended to relationships between groups of individuals, and have shown their value in a number of contexts from kinship relationships in certain primitive tribes to relationships between political parties [4]. These representations are called social networks, also used in political sciences to study international relations, where nodes correspond to nations or group of nations, and the edges join pair of nations that are allied, maintain diplomatic relations, or agree on a particular strategy, among a variety of reasons. Technological networks include the internet, telephone networks, transportation networks and railway systems. The internet is one of the largest man-made networks and can be defined as a huge collection of thousands of millions of computers and routers connected by physical links. Alternatively, at a more elementary level, they can be regarded as consisting of thousands of administrative domains among which data transfer takes place. Biological networks include cellular networks (an ensemble of genes, proteins and other molecules), and the ways in which they interact to regulate cell activities; a biological neural network consisting of functionally related neurons performing a specific physiological function. All of these are relatively small

complex networks compared with the majority of complex networks seen in real life.

Collecting and processing great amounts of data from different systems is a recent technological advance which has facilitated the synthesis of networked systems that resemble, at some point, their natural counterparts in terms of their functional and operational complexity [78]. Since we live in a complex interconnected world, a deeper understanding of the role that those inter-part interactions play in the collective functionality of the systems and in the emergence of different global properties has become very important. "There are people studying the nature of the parts or components of the systems, and there are also people interested in the nature of the connections, but there is a group of people that studies the aspect of the pattern of connections between components (the structure) which is fundamental to the behaviour of the whole system" [86].

When we devise an abstract view of the complex interaction topologies of a system associated with the actors or agents, representing them as nodes and en-coding their interactions as edges, the advantage of applying network science methods to analyse and synthesise these systems becomes clear: the set of tools from network science provides a convenient way for examination of how the structure of the underlying interaction topology among agents evolves into distinct global behaviour. A graph-based abstraction of a complex networked system implies high-level descriptions of the networked topology as nodes and edges, even though certain information about what exactly is shared among the elements of the system is sacrificed.

The last fifteen years have seen significant interest and attention devoted to understanding the structure underlying complex networks, with particular reference to their topologies and the large-scale properties devolving from them. The topology of a complex network is usually represented as a large graph, where each unit of a complex network can be represented by a site (physics), node

(computer science), actor (sociology), or vertex (graph theory) and the connection/interaction between two units may be the equivalent of a bond (physics), link (computer science), tie (sociology) or edge (graph theory). The study of the topological structure of complex networks is one the most fundamental steps for achieving a basic understanding of certain aspects of many kinds of real-world phenomena. Many, if not all, of the properties of the complex system a network it represents can be determined by its structure [36]. The structure of a network always affects its functions, being defined as the "arrangement of and relations between the parts or elements of something complex" or "the way in which the parts of a system or objects are arranged or organised" [36]. The study and understanding of a topological network's structure is also significant in the evaluation and design of networks regulations and protocols that run on top of them. Understanding complex networks' topologies can also protect networks from failures and attacks, with the purpose of achieving a better design and evolution of networks.

The study of complex networks' topologies has not been a simple matter over the past decade, possibly due to the fact that large-scale networks are often a collection of thousands or millions of nodes. In fact, there is no single vantage point from which a complete picture of the topology can be obtained. Besides, complex networks can undergo dramatic changes and constant evolution. For example, it is possible to create or remove a web page on the World Wide Web (WWW) on a daily basis, rendering it difficult to obtain a view of this network. Furthermore, since the network cannot naturally be inspected directly, the task of discovering topologies has fallen to experimentalists developing methods of varying degrees of sophistication to infer its topology from suitable network measurements. The elaborate nature of the network means that there is a great number of possible measurements that can be made, each with its own characteristics: strengths, weaknesses and limitations, and each offering a distinct specific view of the net-

work topology. To achieve a proper understanding of the structure of complex networks, a reference model with which we can compare them is required.

These challenges have prompted the recent use of network models to describe complex systems and has emphasised the study of graph-theoretic properties as a means to characterise the similarities and differences in the structures and the functions of systems over a variety of domains [3, 16, 88]. Researchers have carried out many more studies on the empirical analysis of graph-theoretic properties of real systems, trying to identify unifying properties over numbers of complex networks. Even more attention has been given to developing generic and universal models in an attempt to explain such unifying properties, to infer more properties that are not easily obtained empirically. Many such works implicitly assume that graph theoretic properties adequately capture key system features to serve as a basis for comparison.

0.2 Diffusion in Complex Systems

Diffusion processes are among the most fascinating phenomena in complex networks systems. Diffusion is a fundamental transport process of matter and energy in various physical, chemical and biological systems [71, 130]. Two types of motions are easily observable in nature: smooth, regular motion, such as the Newtonian motion of planets, and random, highly irregular motion, for example the Brownian motion of small specks of dust in the air. The first of these can be predicted and therefore can be described from a deterministic point of view. The second one necessitates a statistical approach. The first man who noted the Brownian motion was the Dutch physician, Jan Ingenhousz in 1794, who, while in the Austrian court of Empress Maria Theresa, observed that finely powdered charcoal floating on an alcohol surface performed a very erratic random motion [32]. The Scottish botanist Robert Brown [18] made a similar observation when

he investigated with a microscope the continuous irregular motion of small particles (micrometers and less in size). The particles moved in disordered trajectories, with no weakening of their motion. They did not depend on the chemical properties of the medium, strengthened as the medium temperature increased, with reduced viscosity and particle sizes. But Brown considered the motion of the particles (which were not atoms of course) as their own property and made no mention of atoms or molecules. Nearly 80 years later, two physicists: Albert Einstein [33] and Marian von Smoluchowski [132], found the physical explanation for Brownian motion, based on taking the thermal motion of molecules surrounding the Brownian particle into account. Seminal papers by Smoluchowski, Einstein and Langevin (see the respective references in [22]), devoted their studies to classical diffusion where the mass density of the grains diffusing in a background medium was related to the stochastic motion of these particles. In usual conditions, such motion of grains leads to a second moment of the mass distribution that grows linearly in time. Diffusion process types of this kind play a crucial role in plasmas, including dusty plasma [122], nuclear physics [125], neutral systems in various phases [44] and a great range of other problems.

At the same time in many systems the deviation from the linear in time dependence of the mean square displacement have been experimentally observed, in particular under essentially non-equilibrium conditions or for some disordered systems. According to Richardson's law, the average square separation of a pair of particles passively moving in a turbulent flow grows with the third power of time [84]. For diffusion typical for glasses and related complex systems [110] the observed time dependence is slower than linear. These two types of anomalous diffusion are characterised as superdiffusion and sub-diffusion. A number of effective models and methods have been suggested in order to describe these two diffusion regimes. Scher and Montroll's continuous time random walk (CTRW) model [116], leading to strong sub-diffusion behaviour, provides a basis for un-

derstanding photoconductivity in strongly disordered and glassy semiconductors. The Lévy-flight model [63], leading to superdiffusion, describing a variety of phenomena as self-diffusion in micelle systems [95], reaction and transport in polymer systems [124] and can be applied even to the stochastic description of financial market indices [45]. For both cases the so-called fractional differential equations in coordinate and time spaces are applied as an effective approach [136]. The history of the further study of Brownian motion is linked with the names of Langevin, Perrin, Fokker, Planck, Uhlenbeck, Ornstein, Chandrasekhar and other well-known physicists [32].

However, for the first time the diffusion equation appeared in Louis Bachelier's thesis [32] (a student of A. Poincaré's). He devoted his thesis, entitled "The theory of speculations", to the study of random processes in the evolution of market prices. It is surprising the way in which the same diffusion equation can describe the behaviour of neutrons in a nuclear reactor, the light in an atmosphere, stock market values on a financial exchange, or particles of flower dust suspended in a fluid. The fact that identical equations describe phenomena completely different in nature directly indicates that the matter concerns the same common quality of a whole class of similar phenomena rather than the concrete mechanism of the phenomenon. The statement of this quality in terms of physical laws and mathematical postulates or definitions enables the liberation of a given pattern from details, not essentially influencing the physical process, and the exploration of the model obtained by means of general laws. This is a typical situation for statistical physics and applied mathematics. The new approaches proposed by Einstein, Smoluchowski and Langevin to describe the Brownian motion, in fact, offer the opportunity to model a considerable variety of natural phenomena. Simultaneously, for mathematicians, whose achievements built the theory of random processes, the Brownian motion became the first object of its application. N. Wiener [137] has contributed in great measure to the mathematical theory of

Brownian motion, insofar as he has proved that the trajectories of the Brownian process almost everywhere are continuous but are not differentiable anywhere. Wiener, Markov, Doob, Kaç, Feller, Bernstein, Lévy, Kolmogorov, Stratonovich, Itô and others [32] studied the mathematical aspects of Brownian motion. Two significant properties are intrinsic to the homogeneous Brownian motion: the diffusion packet initially concentrated at a point later takes on the Gaussian form, whose width grows in time as $t^{1/2}$. This kind of diffusion was termed normal diffusion.

Twenty years after Einstein, Smoluchowski and Langevin's works, L. Richardson published an article [106] presenting empirical data contradicting normal diffusion: the size $\triangle$ of an admixture cloud in a turbulent atmosphere grows in time proportionally to $t^{3/2}$, much more rapidly than in the normal case ($t^{1/2}$). This turbulent diffusion constituted the first example of a superdiffusion process, when $\triangle \propto t^{\gamma}$ with $\gamma > 1/2$. An interpretation of the phenomenon is that it is a diffusion process with a variable diffusivity $D(r) \propto r^{4/3}$. This Richardson's "law of four thirds" was grounded theoretically by the Russian mathematicians A. N. Kolmogorov [66] and A. M. Obukhov [91] as a development from the self-similarity hypothesis of locally isotropic turbulence. However, the fact that the diffusivity should depend not on the coordinates (a turbulent medium is supposed to be homogeneous on average), but on the scale or distance l between a pair of diffusing particles, creates essential difficulties both to finding a solution to the equation and to interpreting it [32]. The particular case when $\gamma = 2$ is known as ballistic diffusion, recognisable by the fact that in short instances the particles are not yet hindered by collisions and diffuse very fast.

There is particularly interest here in the superdiffusive dynamics, found for instance in the diffusion by flows in porous media [96], signal processing [89], and time series statistical analysis of DNA [115]. Others include primary sequences of protein-like copolymers [46], spreading of epidemic processes [52], the flights

of albatrosses [32], animal behaviour and locomotion [120], and financial time series [112]. The superdiffusive processes have been modelled in many different ways (see [79] for a review and analysis). However, the most used models are based on random walks with Lévy flights (RWLF) [32, 80, 121, 131] and on the use of the fractional diffusion equation (FDE)[7, 46, 62, 75, 128]. Although the first method can be easily used for computer simulations, the second is preferred for analytical studies. There are different types of definitions of a fractional derivative, however, such as the Caputo and the Riemann–Liouville fractional operators [99] which then can be interpreted differently adapting differently to the different physical phenomena in conjunction with which they are studied (see [51, 74]). Recently, anomalous diffusion of ultracold atoms has been noted in a discrete one-dimensional system [113]. A simple diffusion model in which the particles are located in real space, each having a velocity which fluctuates in time due to interaction with a bath is the model considered in that work for explaining the superdiffusive process. After some time, the particles' position is distributed in a non-Gaussian manner and the full width at half maximum (FWHM) scales as a power-law of the time with a signature characteristic of superdiffusion.

Dynamical processes which occur on networks are of great significance in order to understand the ways in which complex systems, ranging from the brain to modern man-made infrastructures [9], work. It could be argued that the main reason for the existence of networks is to facilitate the dynamical propagation of effects from one part of a system to another. Despite the fact that there is a considerable number of dynamical processes occurring on networks, diffusion processes are of special importance [14], arising naturally in many social problems where the issue of propagation of information is concerned. Examples include behavioural flocking in popular cultural styles, emotional contagion, collective decision making, the behaviour of pedestrians when they walk and how computer viruses are propagated. Modelling diffusion of materials in a variety of physical

and biological systems can be carried out using analogous models, from the diffusion of water in the brain to the diffusion of oil and gas through rock fractures.

Diffusion processes on networks are described by the equation $\dot{x}(t) = -Lx(t)$, with the initial condition $x(0) = x_0$, where L is the Laplacian operator (which will be defined later on) [123]. For finite networks the Laplacian matrix has been widely studied in the literature due to its relevance in the characterisation of networks structure and dynamics [23, 77]. The Laplacian matrix has been extended to infinite, connected and locally finite graphs and studied as an operator in the Hilbert space over the vertices [19, 49, 57, 58, 61, 123, 135, 138]. However, during the study of dynamical processes on networks, it is generally assumed that information transmission can only take place between one node and its closest neighbours. Recently, a new assumption for the information diffusion in the dynamical processes was presented [35], putting forward that the information can hop from one node to another without it being adjacent. Taking the generalised Laplacian matrix, based on the path matrices that characterise the existence of shortest paths between pairs of nodes in a graph into consideration, allows for modelling the information diffusion. The matrices were brought into being by the problem of determining whether every node of a graph can be visited by means of a process of jumping from one node to another, at distance k from it. A generalisation of the Laplacian matrix — known as the k-path Laplacian and denoted by L_k — which takes into account such long-range hops of the diffusive particle — has recently been considered for finite undirected graphs [35]. However, we should remark that existence of such long-range hops in diffusive processes has been well documented since the 1990s on experimental basis of different nature. First, the group of G. Ehrlich [119] observed experimentally significant contributions to the thermodynamical properties of the self-diffusion of weakly bounded Pd atoms from jumps spanning second and third nearest-neighbours in the metallic surface. Since then, the role of long jumps in atom and molecules diffusing on

metallic surfaces has been confirmed in many different systems [32, 140].

This thesis studies a generalised diffusion equation, which is controlled by the k-path Laplacian operators (LOs), using the transformed generalised k-path LOs for locally finite infinite networks. We stipulate an approach that considers a diffusion process whereby not only nearest neighbour displacements are allowed, but where also some long-range hops in the network are possible. The main result of this work is to develop a new method that accounts for normal and superdiffusive processes on infinite graphs using the $k-$path LOs. For explaining the superdiffusive process, the model utilised is a simple diffusion model where the diffusive particle diffuses in a one-dimensional discrete space, and the particle not only jumps to its nearest neighbours in the $1D$ lattice, but also to any other point in it. The probability scales according to the distance between the two places. The FDE was the mathematical framework employed to describe this anomalous diffusion, resulting in us presenting a new method for description of superdiffusion by a transform of k-path LO defined on an infinite path graph. The k-path LOs allow the derivation of analytical results as the FDE but use a unique framework, very similar to the one traditionally used in graph and network theory. It also makes for an easy computational implementation in the form of a random multi-hopper on graphs [37]. We then investigate some applications of these operators and the transformed ones, and for that we consider the generalised diffusion process. This generalised diffusion equation gives rise to both normal and superdiffusive processes on infinite one-dimensional graphs. Furthermore, we present the generalisation of the problem to the case of the 2-dimensional Cartesian grid. More precisely, we consider the time evolution of the solution of the generalised diffusion equation with initial condition concentrated at one point. We then describe the asymptotic behaviour of the generalized diffusion equation corresponding to the Mellin-transformed k-path Laplacian (which will be defined later on). We then conclude that the superdiffusive process can be obtained for

k-path Laplacian transformed by the Mellin's transform in dimension two.

0.3 Thesis structure

We have structured the present thesis in two main parts which follow the introduction giving an overview on complex networks and graph theory. In part I we present the theoretical background used to build our proposals and analysis, the body of the first part is constituted of 3 chapters. In Chapter 1 we present general concepts from graph theory and operator theory. Chapter 2 presents the essential concepts for the structure of a network that will be relevant to this thesis. Chapter 3 is devoted to review some concepts of dynamical systems that will be useful in this thesis. We show some examples of the possible dynamics that can be modelled on a network, such as normal and anomalous diffusion processes. The second part of the thesis comprises the results and findings coming from our published works. In Chapter 4 we extend the k-path Laplacians L_k to consider connected and locally finite infinite graphs. We then investigate some of the main properties of k-path LOs, such as a self-adjointness and the boundedness of these operators. We also study the transformed k-path LOs using Laplace, factorial and Mellin transforms. In Chapter 5 we study an infinite linear chain and obtain analytical expressions for the transformed k-path LOs as well as for the exponential operators of both, the k-path Laplacians and their transformations. We introduce a new method to describe superdiffusion by a transformation of k-path LOs defined on path graph. In Chapter 6 we study the solutions of the generalized diffusion equation in 2D graphs. In particular, we focus our attention on the *Abstract Cauchy Problem* in an infinite square lattice. Finally, in Chapter 7 we give our conclusions and discuss future work.

Chapter 1

Graph and Operator theories

1.1 Introduction

The purpose of this chapter is to recall some definitions, basic concepts and some theorems which are important for the discussion of our later results. We shall first introduce definitions and notations to cover essential material on graph theory. Then, we are going to cover basics material on operator theory that will be useful throughout this thesis.

1.2 Graph theory

There are many situations when we may use a group of points joined together either by lines or arrows to represent something of our interest. These points may stand for people, places or atoms, and the lines or arrows may be kinship relations, pipelines or chemical bonds. These kinds of diagrams are known under different names: sociograms (psychology), simplexes (topology), circuit diagrams (physics), organisational structures (economics), communication networks (engineering), family trees, etc. [12]. More about graph theory may be found in the literature [17].

Definition 1.1. A graph is the pair of sets $G = (V, E)$ such that $V \neq \phi$ is the set of nodes (or vertices, or points) of the graph G, and $E \subseteq V \times V$ is the set links (or edges, or lines) of G. That is , E consists of those pairs (u, v) for which there is a link from u to v. The vertex set of the graph G will be denoted by $V(G)$ and its edge set by $E(G)$. Therefore $G = (V_G, E_G)$.

In undirected graphs a pair $\{u, v\}$ is usually written as uv (sometimes (u, v)). Notice that then $uv = vu$. In order to simplify notations, we also write $v \in V$ and $e \in E$ instead of $v \in V(G)$ and $e \in E(G)$.

Definition 1.2. For a graph G, we denote

$$n = |V(G)|, \quad m = |E(G)|.$$

The number of vertices n is called the order of G, and m is the size of G.

Definition 1.3. The vertices u and v are adjacent or neighbours, if $uv \in E$. Two edges $e_1 = uv$ and $e_2 = uw$ having a common end, are said to be adjacent with each other.

Definition 1.4. A locally finite graph is a graph in which every vertex has only a finite number of neighbours.

Definition 1.5. A graph $G_s = (V_s, E_s)$ is called subgraph with respect to a given graph $G = (V, E)$ if $V_s \subseteq V$ and $E_s = \{\{v_i, v_j\} \in E / v_i, v_j \in V_s\}$. In other words, the subgraph V_s consists of the vertices in the subset V_s of V and edges in G that are incident to vertices in V_s.

Definition 1.6. A graph in which each edge e is associated with a real number $w(e)$, called its weight, is called a weighted graph. A weighted graph is often written as $G = (V(G), E(G), W(G))$ where $W(G)$ is the set of edge weights.

Definition 1.7. Two graphs G and H are isomorphic, denoted by $G \simeq H$, if there exist bijections $f : V(G) \longrightarrow V(H)$ and $g : E(G) \longrightarrow E(H)$ such that

$$\psi_G(e) = uv \Longleftrightarrow \psi_H(g(e)) = f(u)f(v)$$

for all $u, v \in G$. The pair (f, g) is called an isomorphism between G and H.

1.3 Paths and cycles

Definitions

- A *walk* from node i to node j is an alternating sequence of nodes and edges (a sequence of adjacent nodes) that begins with i and ends with j. The length of the walk is defined as the number of edges in the sequence.
- A *trail* is a walk in which no edge is repeated.
- A *path* is a walk in which no node is visited more than once.
- The walk of minimal length between two nodes is known as *shortest path* or *geodesic*.
- A *cycle* is a closed walk, of at least three nodes, in which no edge is repeated. A *cycle* of length k is usually called a k-cycle and denoted as C_k.
- A graph is said to be connected if, for every pair of distinct nodes i and j, there is a path from i to j, otherwise it is said unconnected or disconnected.
- A graph G that is not connected has two or more connected components that are disjoint and have G as their union.

1.4 Adjacency matrix

An adjacency matrix A is a means of representing which vertices of a graph are adjacent to which other vertices. The adjacency information of the nodes of a graph $G = (V, E)$ can be represented by the adjacency matrix $A = a_{ij}$ defined as:

$$a_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E, \\ \\ 0 & \text{otherwise.} \end{cases} \tag{1.4.1}$$

the dimension of this matrix is $|V| \times |V|$. There exists a unique adjacency matrix for each graph (up to permuting rows and columns) which is not the adjacency matrix of any other graph. This matrix is a symmetric matrix for undirected graphs. In the special case of a finite simple graph, the adjacency matrix is a $(0,1)$-matrix with zeros on its diagonal.

1.5 Incidence matrix

There is another matrix which has a close relation with the adjacency matrix, this is called the incidence matrix.

Definition 1.8. Suppose $G = (V, E)$ is a graph where $V = \{1, 2, \ldots n\}$ and $E = \{e_1, e_2, \ldots, e_m\}$ with $e_i = (u_i, v_i)$. For $1 \leq i \leq m$ and $1 \leq j \leq n$ define

$$b_{ij} = \begin{cases} 1 & \text{if } u_i = j, \\ -1 & \text{if } v_i = j, \\ 0 & \text{otherwise.} \end{cases} \tag{1.5.1}$$

Then the rectangular matrix $B = (b_{ij})$ is called the incidence matrix of G.

1.6 Degree of Vertices

Definition 1.9. Let $v \in G$ be a vertex of a graph G. The neighbourhood of v is the set

$$N_G(v) = \{u \in G \mid vu \in E\}. \tag{1.6.1}$$

The degree of the node v is defined to be

$$k_v = \mid N_G(v) \mid . \tag{1.6.2}$$

The degree k_v is also the number of entries in the vth row or column of the adjacency matrix A of the graph G. It represents the number of nearest neighbours of v. If $k_v = 0$, then v is said to be isolated in G, and if $k_v = 1$, then v is a leaf of the graph. The minimum degree and the maximum degree of G are defined as

$$k_{min}(G) = \min\{k_v \mid v \in G\} \quad and \quad k_{max}(G) = \max\{k_v \mid v \in G\}. \tag{1.6.3}$$

For an undirected graph, the vth row (column) of the adjacency matrix has exactly k_n entries which corresponds to the number of links or nearest neighbours the node v has, this is the degree of the node. The column vector of node degrees k can be obtained from the matrix A and a $|V| \times 1$ all-one vector 1 as follows:

$$k = (1^T A)^T = A1,$$

where 1 is a $|V| \times 1$ column vector with all entries equal to 1 and 1^T its transpose and A is the adjacency matrix of graph G.

The degree matrix K is the matrix which has the node degrees as its main diagonal and is given by

$$K = diag(k). \tag{1.6.4}$$

In addition, The adjacency matrix A, the incidence matrix B and the degree

matrix K are related by the relation

$$A = B^T B - K. \tag{1.6.5}$$

1.7 Special Graphs

Definitions

- A graph $G(V, E)$ is trivial, if it has only one vertex, i.e., $|V(G)| = 1$; otherwise G is nontrivial.

- A graph $G(V, E)$ is simple, if it A has no loops and no two of its edges join the same pair of vertices.

- A graph is k-regular (or regular of degree k) if the degree of each node is k (Fig 1.7.1. a).

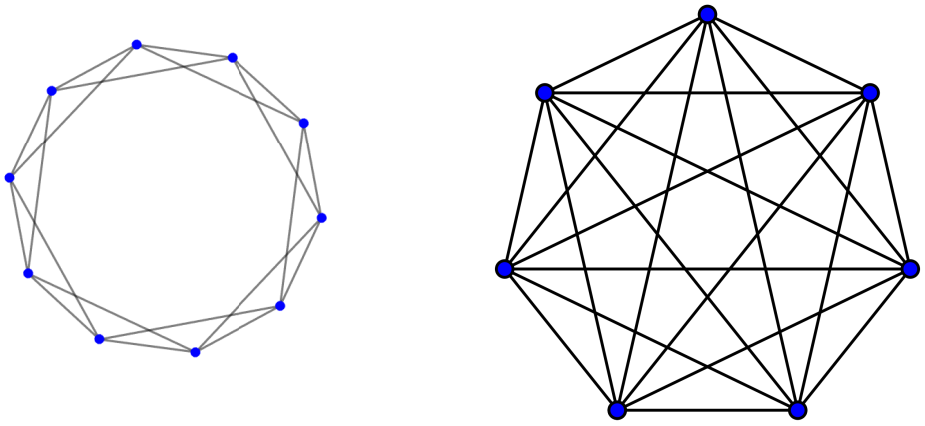
- A complete graph is a graph in which every two vertices are adjacent. The complete graph with n nodes is denoted by K_n (Fig 1.7.1. b).

- The complement of a graph G is the graph $\bar{G}$ created by taking all the nodes in G and joining two nodes whenever they are not linked in G.

- A null graph is a graph with no links. The null graph with n nodes is denoted by N_n. The null graph with n nodes is regular of degree 0 (Fig 1.7.2. a).

- A cycle graph is a graph consisting of a single cycle of vertices and edges. The cycle graph with n nodes is denoted by C_n (Fig 1.7.2. b).

- A bipartite graph is a graph whose set of nodes can be split into two subsets V_1 and V_2 in such a way that each edge of the graph joins a node in V_1 and a node in V_2 (Fig 1.7.2. c).



(a) (b)

Figure 1.7.1: Examples of graphs. (a) Regular graph. (b) Complete graph.

- A star graph S_n is a graph having $(n-1)$ leaves (nodes of degree 1) and one central node having degree $n-1$.
- A tree graph is a connected graph with no cycles. In this graph, any two vertices are connected by exactly one path (Fig 1.7.2. d).

1.8 Operator Theory

This section is devoted to the basic material on operator theory and their basic properties that will be useful through this thesis. There is a vast amount of literature on operator theory, and other advanced topics may be found in the literature [26, 68, 104].

Definition 1.10. Suppose that X is a non-empty set. By a metric or distance function on X, we mean a real-valued function $d : X \times X \longrightarrow \mathbb{R}$ which satisfies the following conditions:

- For every x, $y \in X$, we have $d(x, y) \geq 0$.
- For every x, $y \in X$, we have $d(x, y) = 0 \Longleftrightarrow x = y$.
- For every x, $y \in X$, we have $d(x, y) = d(y, x)$.

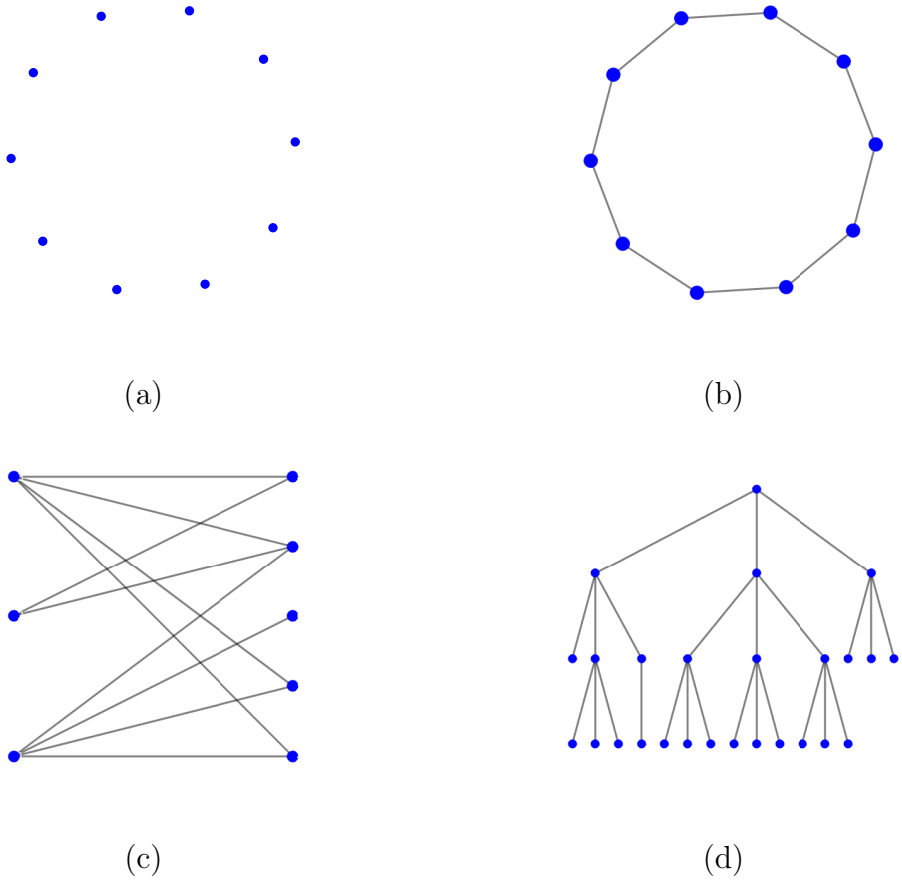


Figure 1.7.2: Examples of graphs. (a) Null graph. (b) Cycle graph. (c) Bipartite graph. (d) Tree

- (Triangle Inequality) For every x, y, $z \in X$, we have $d(x,z) \leq d(x,y) + d(y,z)$.

If these conditions are satisfied, then X is a called a metric space. The number $d(x,y)$ is called the distance from x to y.

Definition 1.11. Suppose that (X,d) is a metric space. A sequence $(x_n)\, n \in \mathbb{N}$ of points in X is said to be a Cauchy sequence if, given any $\varepsilon > 0$, there exists N such that

$$d(x_m, x_n) < \varepsilon \quad \text{whenever } m > n \geq N.$$

Definition 1.12. Suppose that (X,d) is a metric space, and that $M \subseteq X$. We say that M is complete if every Cauchy sequence in M has a limit in M. If X is complete, then we say that the metric space (X,d) is complete.

Definition 1.13. A vector space over a field F is a set M , together with vector addition and scalar multiplication, and satisfying the following conditions:

- For every x, $y \in M$, we have $x + y \in M$.
- For every $x, y, z \in M$, we have $x + (y + z) = (x + y) + z$.
- There exists an element $0 \in M$ such that for every $x \in M$, we have $x + 0 = 0 + x = x$.
- For every $x \in M$, there exists $-x \in M$ such that $x + (-x) = 0$.
- For every x, $y \in M$, we have $x + y = y + x$.
- For every $c \in F$ and $x \in M$, we have $c\,x \in M$.
- For every $c \in F$ and x, $y \in M$, we have $c(x + y) = cx + cy$.
- For every a, $b \in F$ and $x \in M$, we have $(a + b)x = ax + bx$.

- For every$a$, $b \in F$ and $x \in M$, we have $(ab)x = a(bx)$.
- For every $x \in M$, we have $1x = x$.

Definition 1.14. A normed vector space is a vector space N over F, together with a real valued function $\|.\| : N \longrightarrow \mathbb{R}$, called a norm, and satisfying the following conditions:

- For every $x \in N$, we have $x \geq 0$.
- For every $x \in N$, we have $x = 0 \iff x = 0$.
- For every $x \in N$ and every $c \in F$, we have $\|cx\| =\mid c \mid x$.
- (Triangle Inequality) For every x, $y \in N$, we have $\|x + y\| \leq \|x\| + \|y\|$.

Remark 1.15. A norm on N defines a metric d on N which is given by

$$d(x, y) = \|x - y\|,\ x, y \in N,$$

and is called the metric induced by the norm.

Definition 1.16. Suppose that N is a normed vector space over F. Suppose further that N is a complete metric space, i.e., if every Cauchy sequence in N converges to an element of N, under the metric induced by its norm. Then we say that N is a Banach space.

Definition 1.17. By an inner product space, we mean a vector space N over F, together with a function $\langle , \rangle : N \times N \longrightarrow F$, called an inner product, satisfying the following conditions:

- For every $x \in N$, we have $\langle x,\, x\rangle \geq 0$.
- For every x, $y \in N$, we have $\langle x,\, y\rangle = \overline{\langle y,\, x\rangle}$.

- For every $x, y, z \in N$ and all scalars $a, b \in F$, we have $\langle ax + by, z\rangle = a\langle x, z\rangle + b\langle y, z\rangle$.
- For every $x \in N$, we have $\langle x, x\rangle = 0 \iff x = 0$.

Remark 1.18. An inner product on N defines a norm on N given by

$$\| x \| = \sqrt{\langle x, x\rangle} = \langle x, x\rangle^{1/2},\ x \in N,$$

and a metric on N given by

$$d(x, y) = \|x - y\| = \langle x - y, x - y\rangle^{1/2},\ x, y \in N.$$

Definition 1.19. Suppose that N is an inner product space over F. Suppose further that N is a complete metric space under the metric induced by its inner product. Then we say that N is a Hilbert space.

Remark 1.20. Note that every Hilbert space over F is a Banach space over F.

Definition 1.21. Suppose that N is a vector space over F. By a linear operator from N to N, we mean a mapping $L : N \longrightarrow N$ satisfying the following conditions:

- For every $x, y \in N$, we have $L(x + y) = Lx + Ly$.
- For every $c \in F$ and $x \in N$, we have $L(cx) = cLx$.

Remark 1.22. The set of all linear operators on N is denoted by $L(N)$.

Definition 1.23. Suppose that N is normed vector space over F. A linear operator $L : N \longrightarrow N$ is said to be bounded if there exists a real number $M \geq 0$ such that $\|L(x)\| \leq M \|x\|$ for every $x \in N$.

Theorem 1.24. *Suppose that N is a normed vector space over F. Then for any linear operator $L : N \longrightarrow N$, the following statements are equivalent:*

(a) L is continuous in N.

(b) L is continuous at $x = 0$.

(c) L is bounded.

Definition 1.25. Suppose that N is normed vector space over F. We denote by $B(N)$ the collection of all bounded linear operators on N.

Theorem 1.26. *Suppose that N is a Hilbert spaces over F. For every linear bounded operator $L \in B(N)$, there exists a unique linear operator $L^* \in B(N)$ such that $\langle L(x), y\rangle = \langle x, L^*(y)\rangle$ for every $x, y \in N$.*

Remark 1.27. The unique linear operator $L^* \in B(N)$ satisfying the conclusion of Theorem above is called the adjoint operator of the linear operator $L \in B(N)$.

Definition 1.28. A bounded operator L is called self-adjoint if $L = L^*$.

Definition 1.29. Let N be a complex Hilbert space. A bounded self-adjoint linear operator $L : N \to N$ is said to be positive, written $L \geq 0$, if

$$\langle Lx, x\rangle \geq 0,$$

for all $x \in N$.

Definition 1.30. A densely defined linear operator L from one Hilbert space, N_1, to another one, N_2, is a linear operator that is defined on a dense linear subspace $D(L)$ of N_1 and takes values in N_2, written $L : D(L) \subseteq N_1 \to N_2$.

Definition 1.31. Let L and S be operators on N. If $G(L) \subset G(S)$, then L is said to be an extension of S and we write $L \subset S$. Equivalently, $L \subset S$ if and only if $D(L) \subset D(S)$ and $Lx = Sx$ for all $x \in D(L)$.

Definition 1.32. An operator L is closable if it has a closed extension. Every closable operator has a smallest closed extension, called its closure, which we denote by $\overline{L}$.

The notation of adjoint operator can be extended to the unbounded case.

Definition 1.33. Let $L : D(L) \to N$ be a densely defined linear operator in a complex Hilbert space N. Then the Hilbert-adjoint operator $L^* : D(L^*) \to N$ of L is defined as follows. The domain $D(L^*)$ of L^* consists of all $y \in N$, such that there is a $y^* \in N$ satisfying

$$\langle Lx, y\rangle = \langle x, y^*\rangle,$$

for all $x \in D(L)$. The Hilbert-adjoint operator L^* is defined in terms of that y^* by

$$y^* = L^*y.$$

Definition 1.34. A densely defined operator L on a complex Hilbert space is called symmetric (or Hermitian) if $L \subset L^*$, that is, if $D(L) \subset D(L^*)$ and $Lx = L^*x$ for all $x \in D(L)$.

Definition 1.35. A densely defined operator L on a complex Hilbert space is called self-adjoint if $L = L^*$, that is, if and only if L is symmetric and $D(L) = D(L^*)$.

Definition 1.36. A symmetric operator L is said to be essentially self-adjoint if the closure of L ($\overline{L}$) is self-adjoint. Equivalently, L is essentially self-adjoint if it has a unique self-adjoint extension.

Definition 1.37. Let N_1 and N_2 be a Hilbert spaces, L a bounded linear operator from N_1 to N_2. The set of vectors $x \in N_1$ so that $Lx = 0$ is called the kernel of L, written $Ker\, L$. The set of vectors $y \in N_2$ so that $y = Lx$ for some $x \in X$ is called the range of L, written $Ran\, L$.

Notice that both $Ker\, L$ and $Ran\, L$ are subspaces. $Ker\, L$ is necessarily closed, but $Ran\, L$ may not be closed.

Definition 1.38. The identity operator $I_x : N \to N$ is defined by $I_N x = x$ for all $x \in N$. We also write simply I for I_x; thus, $Ix = x$.

Theorem 1.39. *[104] Let L be a symmetric operator on a Hilbert space N. Then the following are equivalent:*

1. L is self-adjoint.
2. L is closed, $Ker(L^* + I) = \{0\}$ and $Ker(L^* - I) = \{0\}$.
3. $Ran(L + I) = N$ and $Ran(L - I) = N$.

Proposition 1.40. *[104] Let L be a symmetric operator on a Hilbert space. Then the following are equivalent:*

1. L is essentially self-adjoint.
2. $Ker(L^* + I) = \{0\}$ and $Ker(L^* - I) = \{0\}$.
3. $Ran(L + I)$ and $Ran(L - I)$ are dense.

Proposition 1.41. *[117] Let L be a symmetric operator on a Hilbert space N and non-negative , i.e.*

$$\langle Lx, x\rangle \geq 0,$$

for all $x \in D(L)$. Then the following are equivalent:

1. L is self-adjoint.
2. L is closed and $Ker(L^* + I) = \{0\}$.
3. $Ran(L + I) = N$

Proposition 1.42. *[34] Let L be a bounded operator. Then the unique solution of the Cauchy problem*

$$u'(t) = -Lu(t),\ u(0) = u_0,$$

is given by the semigroup applied to the initial condition, i.e.,

$$u(t) = T(t)u_0,$$

and that the semigroup is given by the series

$$T(t) = e^{-tL} = \sum_{n=0}^{\infty} \frac{(-t)^n}{n!} L^n.$$

Let us briefly recall the definition of the polylogarithm and then consider some properties that help us to prove some lemmas in the following chapters in this thesis.

Definition 1.43. [93, 25.12.10] For real or complex s and z the polylogarithm $Li_s(z)$ is defined by

$$Li_s(z) := \sum_{k=1}^{\infty} \frac{z^k}{k^s}, \qquad |z| < 1, \tag{1.8.1}$$

and by analytic continuation to $\mathbb{C} \setminus [1, \infty)$ with 1 being a branch point. The special case $z = 1$ is the Riemann zeta function:

$$Li_s(1) = \zeta(s) = \sum_{k=1}^{\infty} \frac{1}{k^s}, \tag{1.8.2}$$

Remark 1.44. [93, 25.12.12] We have

$$Li_s(z) = \Gamma(1-s)(\ln \frac{1}{z})^{s-1} + \sum_{n=0}^{\infty} \zeta(s-n) \frac{(\ln z)^n}{n!}, \; s \neq 1, 2, 3, \ldots, |\ln z| < 2\pi. \tag{1.8.3}$$

Remark 1.45. [72, p. 131] We have

$$Li_s(z) = \frac{(\ln z)^{s-1}}{(s-1)!}(1 + \frac{1}{2} + \ldots + \frac{1}{s-1} - \ln(\ln \frac{1}{z})) + \sum_{n=0, n \neq s-1}^{\infty} \zeta(s-n) \frac{(\ln z)^n}{n!}. \tag{1.8.4}$$

Theorem 1.46. *(Dominated Convergence Theorem) Suppose* $f_n : \mathbb{R} \to [-\infty, \infty]$

are (Lebesgue) measurable functions such that the pointwise limit $f(x) = \lim_{n\to\infty} f_n(x)$ *exists. Assume there is an integrable* $g : \mathbb{R} \to [0, \infty]$ *with* $\mid f_n(x) \mid \leq g(x)$ *for each* $x \in \mathbb{R}$. *Then* f *is integrable as is* f_n *for each* n, *and*

$$\lim_{n\to\infty} \int_{\mathbb{R}} f_n d\mu = \int_{\mathbb{R}} \lim_{n\to\infty} f_n d\mu = \int_{\mathbb{R}} f d\mu.$$

Chapter 2

Network Structure

2.1 Introduction

Graph theory is the natural framework for the exact mathematical treatment of complex networks and, formally, a complex network can be represented as a graph [15]. The words graph and network have been used imprecisely in practice due to the close relationship between graph theory and network theory. Graph theory and network theory principally differ from each other in that in the first, the whole graph is given exactly, then initiating the search for relationships between its parameters, variables and functions or for efficient algorithms for their computation. In contrast, for every large real-world network, variables are typically not entirely known and probably not well defined, which makes representing them as infinite graphs to promote effective analysis appropriate. Interest in the theory of networks has increased recently, accompanied by development among different scientific sectors, producing several works in an attempt to compress all this knowledge into a general framework.

The purpose of this chapter is to provide material in a brief account of the latest developments in the characterisation of a network's structural properties. The study will only cover very immediate areas as there is a considerable quantity

of literature relating to network structures and dynamics and other advanced topics [36, 86]. Therefore, the essential concepts for the structure of a network, relevant to this thesis will be presented. A variety of different scientific areas in related literature exists for studies of graph and network theories [15].

2.2 A formal definition of Networks

The study of networks is related to graph theory, and so we will sometimes use the terms graph and network interchangeably. However, network theory relies not only on graph theory, but also makes use of topics such as statistical mechanics, geometry, topology, and dynamical systems.

Definition 2.1. A network is a triple $G = (V, E, f)$ where V is a finite set of vertices or nodes, $E \subseteq V \times V = \{e_1, e_2, ..., e_m\}$ is a set of edges or links and f is a mapping which associates some elements of E to a pair of elements of V, such as that if $v_i \in V$ and $v_j \in V$ then $f : e_p \longrightarrow [v_i, v_j]$ and $f : e_p \longrightarrow [v_j, v_i]$; and a weighted network is the triple $G = (V, E, f)$ defined by replacing the set of edges E by a set of edges weights $W = \{w_1, w_2, ..., w_m\}$ such that $w_i \in \mathbb{R}$. There are different kinds of networks [36, 86] that includes:

- Computer Networks: The Internet topology (at both the Router and the Autonomous System (AS) levels) is a graph, with edges connecting pairs of routers/AS. This is a graph, which can be both weighted or unweighted.

- Ecology: Food webs are graphs with each node representing a species, and the species at one endpoint of an edge eats the species at the other endpoint.

- Biology: Protein interaction networks link two proteins if both are necessary for some biological process to occur.

- Sociology: Individuals are the nodes in a social network edges representing ties (with labels such as friendship, business relationship, trust, etc.)

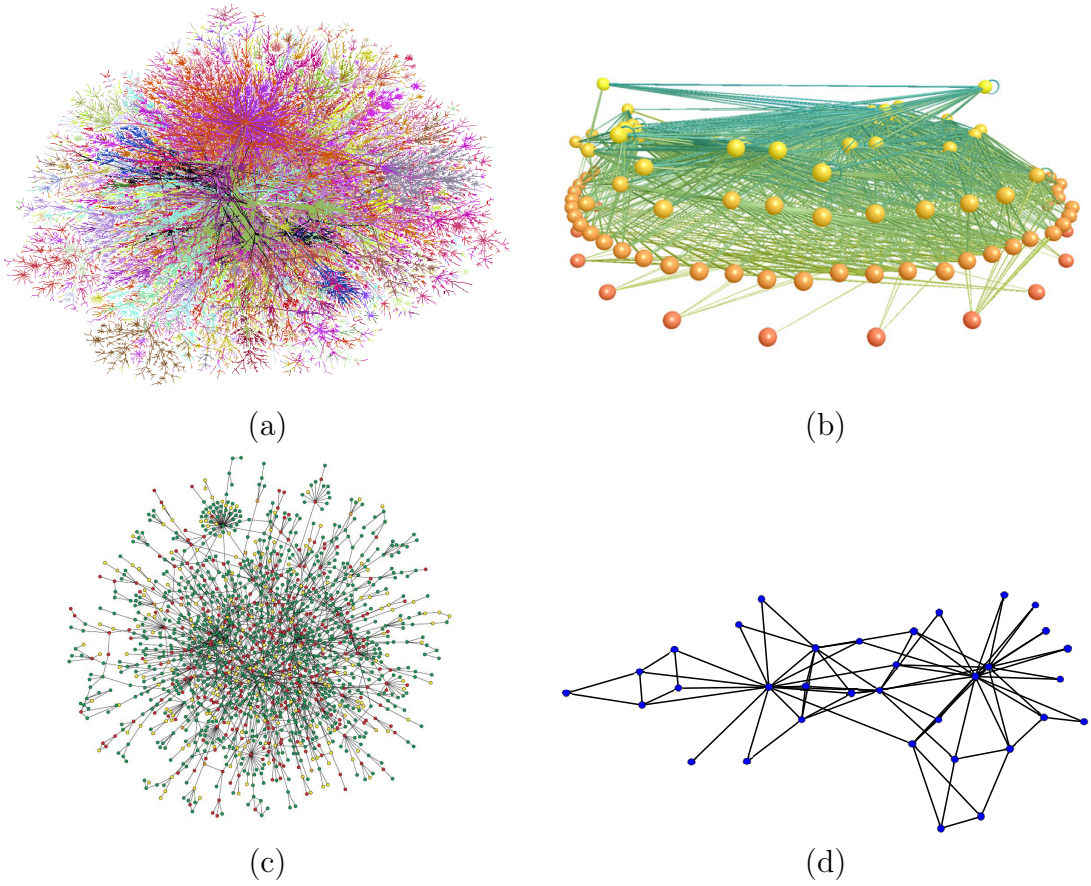


Figure 2.2.1: Some examples of networks. (a) Internet networks [86]. (b) Food web network [86]. (c) Protein-Protein interaction network [53]. (d) Friendship network.

between people.

- User Psychology: Click stream graphs are bipartite graphs connecting internet users to the websites they visit, thus encoding some information about the psyche of the web user.

2.3 Properties of Networks

2.3.1 Degree Distributions

From the information that the node degrees of a network provide, some important insights into the structure of the entire network can be revealed. This analysis

is based on the distribution of node degrees in the network and such degree distribution forms the most fundamental topological characterisation of a network. The degree distribution may be found in terms of the probability $p(k)$, defined as the probability that a node chosen uniformly at random has degree k, or equivalently as the fraction of nodes in the graph having degree k. Alternatively, the degree distribution is denoted as $p(k)$, indicating that the variable k assumes non-negative integer values. The probability $p(k)$ is given by

$$p(k) = \frac{n(k)}{n}, \tag{2.3.1}$$

where $n(k)$ is the number of nodes having degree k in a network of size n. Some important information, but not all, about the network can be obtained from the degree distribution. Information on how the degree is distributed among the nodes of an undirected network can be gained either by a plot of $n(k)$ versus the degree k, often in log-log scale, providing a qualitative idea about the kind of statistical distribution followed by the node degrees or by the calculation of the moments of the distribution. The n-moment of $p(k)$ is defined as follows:

$$< k^n >= \sum_k k^n p(k). \tag{2.3.2}$$

The first moment $< k >$ (sometimes written $\bar{k}$) is the mean degree of the network. The second moment $< k^2 >$, called the variance, measures the fluctuations of the connectivity distribution. In the limit of infinite graph size, $< k^2 >$ radically changes the behaviour of the dynamical processes occurring throughout the network. Among the different kinds of degree distributions in the study of complex networks there are the Poisson distribution, the Gaussian distribution, the power-law distribution and the exponential distribution (Fig 2.4.1). Two distributions, the in-degree distribution of node $p(k^{in})$ with $k_i^{in} = \sum_j a_{ji}$ and the out-degree distribution of $p(k^{out})$ with $k_i^{out} = \sum_j a_{ij}$ should be taken into account in the case

of directed networks.

2.4 Power-Law Degree Distribution

One of the degree distributions that has attracted the attention of the scientific and even popular literature is the power-law degree distribution. The characteristic of this distribution is that the probability of finding a node with degree k decreases as a negative power of the degree. Its expression is $p(k) \sim k^{-\gamma}$ meaning that the probability of finding a high-degree node is relatively small compared with the high probability of finding low-degree nodes. Networks showing this form of degree distribution are known as "scale-free" networks, referring to the existence of a power-law relation

$$p(k) \sim Ak^{-\gamma},$$

between the probability density function and the node degree which, when scaling the degree by a constant factor c, results in a proportionate scaling of the function, i.e.

$$p(k, c) = A(ck)^{-\gamma} = Ac^{-\gamma}p(k),$$

which is identical to $p(k)$ except for a change of scale.

It is possible to represent power-law relations on a logarithmic scale, resembling a straight line of the form

$$\ln p(k) = -\gamma \ln k + \ln A,$$

where $-\gamma$ is the slope and $\ln A$ is the intercept of the function. When $p(k)$ vs k in a log-log scale (Fig 2.4.2) is plotted, the tail of the distribution is frequently

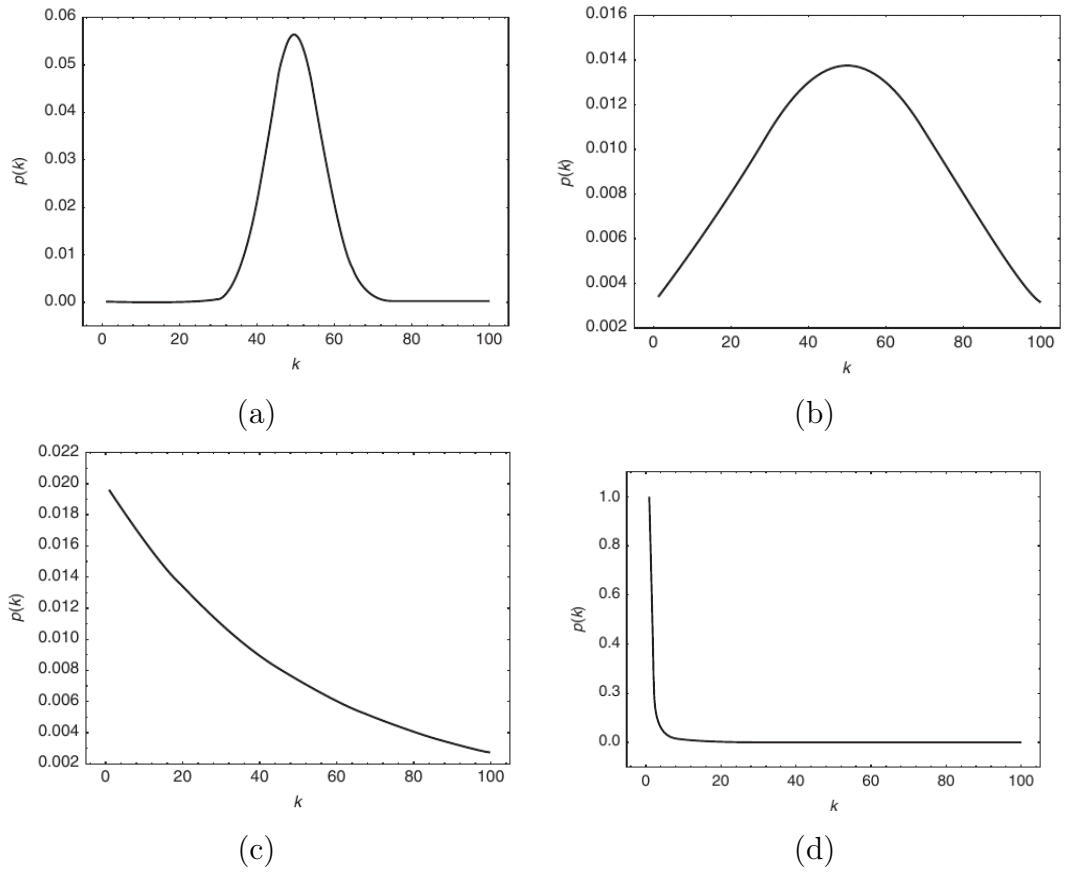


Figure 2.4.1: Some examples of degree distribution in networks. (a) Poisson distribution. (b) Gaussian distribution. (c) Exponential distribution. (d) Power-law distribution [36].

very noisy. The cumulative distribution function (CDF) approach, defined as

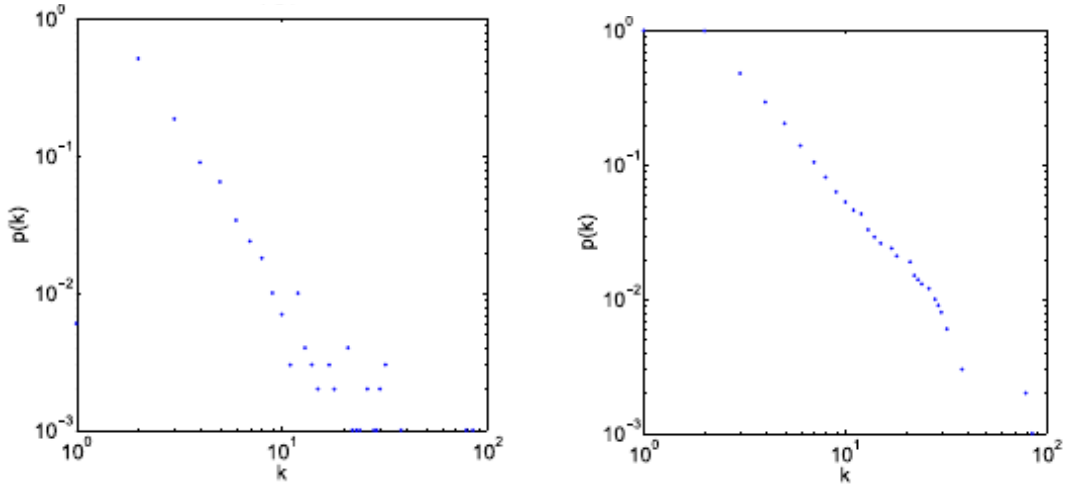
$$P(k) = \sum_{k'=k}^{\infty} p(k'),$$

can be employed to reduce such noise, and represents the probability of choosing a node with degree greater than, or equal to k at random.

For the case of power-law degree distributions $P(k)$ also exhibits a power-law decay of the form

$$P(k) \sim \sum_{k=k'}^{\infty} k'^{-\gamma} \sim k^{-(\gamma-1)},$$

this means that the log-log plot of $P(k)$ vs k will be a straight line too for the scale-free networks.



(Probability) (Cumulative)

Figure 2.4.2: Probability and cumulative distribution functions of a network with power-law degree distribution [36].

2.5 Continuous Distributions

We now consider some of the more important continuous probability distributions.

2.5.1 The Normal Distribution

The most widely known and used of all distributions is the normal distribution. It is important insofar as a great many random variables of interest, in all areas of the physical sciences and beyond, are described either exactly or approximately by a Gaussian distribution. Furthermore, other, more complicated, probability distributions can be approximated using the Gaussian distribution.

If X is normally distributed with a mean μ and standard deviation σ, we write $X \sim N(\mu, \sigma^2)$, μ and σ being the parameters of the distribution. The probability density of the Normal distribution is given by

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp[-(x-\mu)^2/2\sigma^2], \ -\infty < x < \infty.$$

The Normal distribution is symmetric about the point $x = \mu$ and is characterised by the 'bell' shape shown in Figure 2.5.1. Changing μ and σ has the effect only

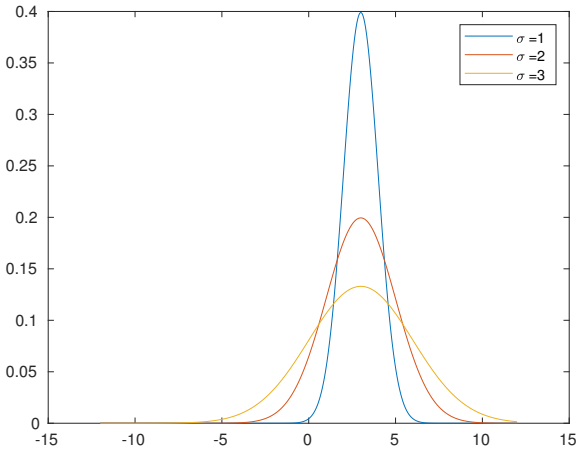


Figure 2.5.1: The normal distribution for mean $\mu = 3$ and different values of the standard deviation σ.

of shifting the curve along the x-axis or broadening or narrowing it, respectively. Thus a change of origin and scale can reduce all Gaussians to a standard form of equivalence. We therefore consider the random variable $Z = \frac{(X-\mu)}{\sigma}$, for which the probability density function takes the form

$$\phi(z) = \frac{1}{\sqrt{2\pi}} \exp(-z^2/2),$$

termed the standard Gaussian distribution and has a mean $\mu = 0$ and variance $\sigma^2 = 1$. The random variable Z is called the standard variable.

2.5.2 The Cauchy Distribution

The canonical example of a "pathological" distribution, as both its mean and its variance are undefined, is the Cauchy distribution, often employed in statistics. It does not have finite moments of an order greater than or equal to one; only fractional absolute moments exist. The Cauchy distribution $f(x; x_0, \gamma)$ is the distribution of the X-intercept of a ray issuing from (x_0, γ) with a uniformly distributed angle. It is significant in physics as the result of being the solution to the differential equation describing forced resonance. In mathematics, it is

closely related to the Poisson kernel, which is the fundamental solution for the Laplace equation in the upper half-plane. In spectroscopy, it is the description of the shape of spectral lines which are subject to homogeneous broadening where all atoms interact in the same way with the frequency range contained in the line shape. Homogeneous broadening, particularly collision broadening, is caused by a number of mechanisms, and is one of the few distributions that is stable and has a probability density function that can be expressed analytically, the others being the normal distribution and the Lévy distribution.

The Cauchy distribution has the probability density function

$$f(x; x_0, \gamma) = \frac{1}{\pi\gamma[1 + (\frac{x-x_0}{\gamma})^2]} = \frac{1}{\pi\gamma}[\frac{\gamma^2}{(x - x_0)^2 + \gamma^2}],$$

where x_0 is the location parameter, specifying the location of the peak of the distribution, and γ is the scale parameter which specifies the half-width at half maximum ($HWHM$), alternatively 2γ is full width at half maximum ($FWHM$). Also, γ is equal to half the interquartile range and is sometimes termed the probable error. The special case is when $x_0 = 0$ and $\gamma = 1$ and is called the standard Cauchy distribution with the probability density function [109, 8]:

$$f(x; 0, 1) = \frac{1}{\pi(1 + x^2)}.$$

2.6 Stable Distribution

Stable distributions are a rich class of distributions that include the Gaussian and Cauchy distributions in a family that allows skewness and heavy tails. The class was characterised by Paul Lévy [70] in his study of normalized sums of independent identically distributed terms. The general stable distribution is described by four parameters: an index of stability, a skewness parameter, a scale parameter and a location parameter [90].

Stable distributions have been proposed as a model for many types of physical and economic systems. There are several reasons for using a stable distribution to describe a system. The first is where there are solid theoretical reasons for expecting a non-Gaussian stable model, e.g. reflection of a rotating mirror yielding a Cauchy distribution, hitting times for a Brownian motion yielding a Levy distribution, the gravitational field of stars yielding the Holtsmark distribution. The second reason is the Generalized Central Limit Theorem which states that the only possible non-trivial limits of normalized sums of independent identically distributed terms are stable. It has been argued that many observed quantities are the sum of many small terms – the price of a stock, the noise in a communication system, etc. and hence a stable model should be used to describe such systems [90]. The third argument for modelling with stable distributions is empirical: many large data sets exhibit heavy tails and skewness. The strong empirical evidence for these features combined with the Generalized Central Limit Theorem is used by many to justify the use of stable models. There are examples in finance, economics and communication systems where the data sets are poorly described by a Gaussian model, but possibly can be described by a stable distribution [90]. The stable distribution can be most conveniently described by its characteristic function as follows:

Definition 2.2. A random variable X is said to have a stable distribution if there are parameters $0 < \alpha \leq 2$, $\gamma \geq 0$, $-1 \leq \beta \leq 1$, and $\delta \in \mathbb{R}$ such that its characteristic function has the following form [114]:

$$\phi(z;\alpha,\beta,\gamma,\delta) = \exp\Big[-|\gamma z|^{\alpha}\Big(1 + i\beta\, sign(z)\omega(z,\alpha)\Big) + i\delta z\Big], \qquad z \in \mathbb{R},$$

where

$$\omega(z,\alpha) = \begin{cases} -\tan\dfrac{\pi\alpha}{2} & \text{if } \alpha \neq 1, \\ \dfrac{2}{\pi}\ln|z| & \text{if } \alpha = 1. \end{cases}$$

The parameter α is the index of stability and

$$sign(z) = \begin{cases} 1 & \text{if } z > 0, \\ 0 & \text{if } z = 0, \\ -1 & \text{if } z < 0. \end{cases}$$

The parameters β, γ, and δ are unique (β is irrelevant when $\alpha = 2$).

Thus, a stable characteristic function (or distribution) is completely determined by four parameters: α, β, γ, and δ, where [89]:

1. α is called the characteristic exponent. It is uniquely determined. The characteristic exponent measure the thickness of the tails of the distribution.

2. β is a symmetry parameter. $\beta = 0$ implies that the distribution is symmetric about δ. In this case, the distribution is called symmetric α-stable.

3. γ is a scale parameter, also called the dispersion. It is similar to the variance of the Gaussian distribution and equals half the variance in that Gaussian case (i.e., when $\alpha = 2$).

4. δ is a location parameter. For symmetric stable distribution, it is the mean when $1 < \alpha \leq 2$ and median when $0 < \alpha < 1$.

The distribution function and density of the stable distribution with characteristic function $\phi(z; \alpha, \beta, \gamma, \delta)$ are denoted by $S(\alpha, \beta, \gamma, \delta)$ and $f(\xi; \alpha, \beta, \gamma, \delta)$ respectively, where

$$f(\xi; \alpha, \beta, \gamma, \delta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \phi(z; \alpha, \beta, \gamma, \delta) e^{i\xi z} dz.$$

In the applications in the latter sections we only interested in the case when $\beta = \delta = 0$, which yields the following simpler function

$$\phi(z; \alpha, 0, \gamma, 0) = \exp(-|\gamma z|^{\alpha}).$$

As well, the parameters α and γ that will be used depends on the parameter s in the Mellin transformation. We also used the scale parameter γ to specify the full width at half maximum ($FWHM$).

There are two special cases where the density f can be computed explicitly: when $\alpha = 2$, we obtain a normal distribution with variance $2\gamma^2$, i.e.

$$f(\xi; 2, 0, \gamma, 0) = \frac{1}{2\sqrt{\pi}\,\gamma} \exp\Big(-\frac{\xi^2}{4\gamma^2}\Big);$$

when $\alpha = 1$, we obtain a Cauchy distribution:

$$\begin{aligned} f(\xi; 1, 0, \gamma, 0) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-|\gamma z|} e^{i\zeta z} dz \\ &= \frac{1}{2\pi} [\int_{-\infty}^{0} e^{-\gamma z} e^{i\zeta z} dz + \int_{0}^{\infty} e^{\gamma z} e^{i\zeta z} dz] \\ &= \frac{1}{2\pi} (\frac{1}{\gamma + i\zeta} + \frac{1}{\gamma - i\xi}) \\ &= \frac{1}{\pi} \cdot \frac{\gamma}{\gamma^2 + \xi^2}. \end{aligned}$$

When $\alpha < 2$, Nolan [90] has shown that the tails of non-Gaussian stable distributions are asymptotically equivalent to a Pareto law. Specifically, if X is a standardized stable random variable with characteristic exponent $0 < \alpha < 2$ and skewness parameter $-1 \leq \beta \leq 1$, then as $x \to \infty$,

$$P(X > \zeta) \sim \gamma^\alpha c_\alpha (1 - \beta) \zeta^{-\alpha},$$

$$f(\zeta/\alpha, \beta, \gamma, \delta; 0) \sim \alpha \gamma^\alpha c_\alpha (1 - \beta) \zeta^{-(\alpha+1)},$$

where $c_\alpha = \Gamma(\alpha)\, \sin(\frac{\pi\alpha}{2})/\pi$.

Thus, the density has a power-like decay:

$$f(\xi; \alpha, 0, \gamma, 0) \sim \frac{1}{\pi} \Gamma(\alpha + 1) \sin\Big(\frac{\pi\alpha}{2}\Big) \gamma^\alpha \cdot \frac{1}{\xi^{\alpha+1}} \qquad \text{as } \xi \to \pm\infty. \tag{2.6.1}$$

2.7 The central limit theorem (CLT)

The central limit theorem states that the sum of a number of independent and identically distributed random variables with finite variances will tend to a normal distribution as the number of variables grows. More precisely, let X_i, $i = 1, 2, \ldots, n$, be independent random variables, each of which is described by a probability density function $f_i(x)$ with a mean μ_i and a variance σ_i^2. The random variable $\bar{X} = \frac{(\sum_i X_i)}{n}$, i.e. the 'mean' of the X_i, has the following properties:

1. its expectation value is given by $E[\bar{X}] = (\sum_i \mu_i)/n$;
2. variance is given by $V[\bar{X}] = (\sum_i \sigma_i^2)/n^2$;
3. as $n \longrightarrow \infty$ the probability function of $\bar{X}$ tends to a Gaussian with corresponding mean and variance.

We note that for the theorem to hold, the probability density functions $f_i(x)$ must possess formal means and variances. Thus, for example, if any of the X_i were described by a Cauchy distribution then the theorem would not apply.

2.8 The mean square displacement (MSD)

Although it was Jan Ingenhousz who made the first known documented observations of fluctuating movements of carbon dust particles in alcohol in 1765, Robert Brown is credited with the discovery of Brownian motion due to his observations of pollen in water in 1827. Also because the previous description by Ingenhousz was not well known, the chaotic movement was for a long time considered to be a property of living or at least organic matter. Brownian motion is stochastic movement of small particles suspended in a solution. The molecules (for example water molecules) constituting the fluid constantly hit the immersed objects which results in chaotic and non-directed movements. These movements can be measured by the mean square displacement $<\mid x \mid^2>$ and the lag time: $\triangle t$, and

are characterised by the diffusion coefficient D which is a measure of the speed of diffusion [102].

The mean square displacement (MSD) of a set of N displacements x_n is given by

$$<\mid x \mid^2>= \frac{1}{N}\sum_{k=1}^{N} \mid x_k \mid^2 .$$

It occurs particularly in Brownian motion and random walk problems.

2.9 Shortest paths

A shortest path, also called a geodesic path, is a minimum path distance between two vertices. Shortest paths fulfil a significant role in transport and communication within a network. If it is necessary to send a data packet from one computer to another through the Internet, the geodesic path provides an optimal path way, resulting in a fast transfer and saving system resources [98]. The average shortest path length, also known as characteristic path length, defined as the mean of geodesic lengths over all pairs of nodes [97, 133] provides a measurement of the typical separation between two nodes in the graph, thus:

$$l = \frac{1}{n(n-1)} \sum_{i,j \in V, i \neq j} d_{ij},$$

where n is the number of nodes and d_{ij} is the shortest distance between nodes i and j. We denote a shortest-path of length l between v_i and v_j as $P(v_i, v_j)$. The nodes v_i and v_j are called the endpoints of the path.

In a real network like the World Wide Web (WWW), the quick transfer of information and reduced costs are facilitated by a short average path length. Studying average path length is a way of evaluating the efficiency of mass transfer in a metabolic network. Fewer losses will occur in a power grid network if its average path length is minimised. For reasons such as this, shortest paths have

also fulfilled an important role in the characterisation of the internal structure of a graph [133, 134]. In the case of an undirected network, the shortest path lengths can be represented in a square symmetric matrix D in which the entry d_{uv} is the length of the geodesic from node u to node v. Where directed networks are concerned, D is not necessarily symmetric and it may contain entries equal to infinity [36].

Definition 2.3. The maximum graph distance between u and any other vertex v of the network is called the eccentricity and is defined as

$$e(u) = \max_{v \in V(G)} \{d(u, v)\}.$$

Definition 2.4. The maximum value of d_{uv} (the maximum eccentricity) is called the diameter of the network, and is defined as

$$d_{\max} = \max_{u,v \in V(G)} \{d(u, v)\}.$$

Definition 2.5. The minimum graph eccentricity is called the graph radius.

Definition 2.6. A node is called central if its eccentricity is equal to the radius of the network, and the centre of the graph is constituted by the set of all central nodes.

Definition 2.7. The sum of all entries of a row (column) of the distance matrix D is referred to as the distance sum of the correspondent node, and is defined as

$$D = \sum_{v \in V(G)} d(u, v). \tag{2.9.1}$$

It is also known as the total distance or status of the node.

2.10 Laplacian matrix of a network

It is possible that the first recognisable appearance of the Laplacian matrix is in what has become known as Kirchhoff's matrix tree theorem, referred to variously as Kirchhoff matrix, matrix of admittance, information matrix, Zimm matrix, Rouse-Zimm matrix, connectivity matrix and vertex-vertex incidence matrix, depending on the field of application [77]. It is also possible that the origins of the justification of the name 'Laplacian' comes from a study of vibrations of membranes concerned with the question of whether one could "hear the shape of a drum" posed by Mark Kac in 1966 [77, 59]. This matrix is important for the study of networks because of the application of its spectral properties to tackle problems such as clustering, pattern recognition, consensus algorithms, synchronisation, information theory, or expanders, among others [35].

Definition 2.8. The matrix L whose entries are defined as follows:

$$L(i,j) = \begin{cases} k_i & \text{if } i = j, \\ -1 & \text{if } i \text{ and } j \text{ are adjacent}, \\ 0 & \text{otherwise}, \end{cases} \tag{2.10.1}$$

where k_i are the degrees of the vertices, is called the Laplacian matrix of the network.

If K is the diagonal matrix whose entries are the degrees of the vertices of the network, i.e.

$$K(i,j) = \begin{cases} k_i & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases} \tag{2.10.2}$$

Then, The graph Laplacian can also be written in terms of the adjacency matrix by taking into account (2.10.1) as

$$L = K - A, \tag{2.10.3}$$

being A the adjacency matrix of the graph G and K the degree matrix of the same graph.

2.10.1 The Normalised Laplacian

The normalised Laplacian may have a different form depending on the normalisation factor chosen. Here are examples of two different normalised Laplacian matrices.

- The normalised Laplacian denoted by $\mathcal{L}$ whose entries are given by:

$$\mathcal{L}(i,j) = \begin{cases} 1 & \text{if } i = j \text{ and } d_i \neq 0, \\ -\dfrac{1}{\sqrt{d_i d_j}} & \text{if } i \text{ and } j \text{ are adjacent}, \\ 0 & \text{otherwise.} \end{cases} \tag{2.10.4}$$

- The normalised Laplacian denoted Δ whose entries are given by:

$$\Delta(i,j) = \begin{cases} 1 \quad if & i = j \text{ and } d_i \neq 0, \\ -\dfrac{1}{d_j} \quad if & i \text{ and } j \text{ are adjacent}, \\ 0 & \text{otherwise.} \end{cases} \tag{2.10.5}$$

The relationship between the normalised Laplacian $\mathcal{L}$, the degree matrix K and the Laplacian L is given by:

$$\mathcal{L} = K^{-1/2} L K^{-1/2}, \tag{2.10.6}$$

$$= I - K^{-1/2} A K^{-1/2}, \tag{2.10.7}$$

where I is the identity matrix and the matrix $K^{-1/2}$ is such that $K^{-1/2} = \frac{1}{\sqrt{d_i}}$. We also have a similar relationship involving the normalised Laplacian Δ

$$\Delta = K^{-1/2}\mathcal{L}K^{-1/2}. \tag{2.10.8}$$

There are interesting properties of the Laplacian matrix of a network can be found in [36].

2.11 Spectral analysis of networks

The study of spectral properties of adjacency matrices represents an entire or research in algebraic theory. The study of spectral properties of matrices representing graphs that we know as spectral graph theory [78] has evolved. This branch of graph theory focuses on the study of the eigenvalues associated with the matrix representation of graphs. With reference to the Laplacian matrix, important properties for dynamical problems in networks [35] can be shown in its spectrum and eigenvalues.

The spectrum of a network is the set of the eigenvalues of its adjacency matrix A and their multiplicities. Suppose there are p distinct eigenvalues;

$$\mu_1(A) > \mu_2(A) > \ldots > \mu_n(A),$$

and let

$$m(\mu_1(A)), m(\mu_2(A)), \ldots, m(\mu_p(A)),$$

be their multiplicities, i.e., the number of times each of them appears as an eigenvalue of A. Then, the spectrum of A is written as

$$Sp(A) = \{\mu_1(A)^{m(\mu_1(A))}, \ldots, \mu_p(A)^{m(\mu_p(A))}\}. \tag{2.11.1}$$

The eigenvalues of the adjacency matrix A are the zeros of the characteristic polynomial of the network, $\det(\mu I - A)$, and the numbers μ satisfy the equation

$$Au = \mu(A)u, \tag{2.11.2}$$

where each non-zero vector u is called an eigenvector of A. The adjacency matrix A is real and symmetric, in the case of simple undirected networks, therefore its eigenvalues $\mu_1(A) \geq \mu_2(A) \geq \ldots \geq \mu_n(A)$ are real and the associate eigenvectors are orthogonal. The largest eigenvalue of the adjacency matrix A is called the index of the network or its spectral radius denoted by $\rho(A)$. Here are some spectra of some particular networks [36]:

1. Path, $P_n : \mu_j(A) = 2\cos(\pi j/n + 1)$, $j = 1, \ldots n$.
2. Cycle, $C_n : \mu_j(A) = 2\cos(2\pi j/n)$, $j = 1, \ldots n$.
3. Star, $S_n : Sp(A) = \{\sqrt{n}, 0^{n-2}, -\sqrt{n}\}$.
4. Complete, $K_n : Sp(A) = \{(n-1)^1, -1^{n-1}\}$.
5. Complete bipartite, $K_{n_1,n_2} : Sp(A) = \{-\sqrt{n_1 n_2}, 0^{n_1+n_2-2}, \sqrt{n_1 n_2}\}$.

In accordance with the Perron-Frobenius Theorem [40], if $\mu_1(A)$ is the index of a connected undirected network, then it has multiplicity equal to one. Its associate eigenvector, called the principal eigenvector, is positive. Let $\bar{k}$, $k_{\min}$ and $k_{\max}$ be the range, minimum, and maximum degree, respectively, in a network. Then, the index of the network is bounded as follow:

$$k_{min} < \bar{k} < \mu_1(A) < k_{max}.$$

The latter holds only if the network is regular. The index of any network satisfies

the following inequality:

$$2\cos\frac{\pi}{n+1} \leq \mu_1(A) \leq n-1, \tag{2.11.3}$$

where the lower bound is obtained for the path P_n and the upper one is obtained for the complete network K_n [36].

Similar to the network spectrum based on the adjacency matrix, the spectrum of the Laplacian matrix is given by:

$$Sp(L) = \begin{pmatrix} \mu_1(L) & \mu_2(L) & \dots & \mu_n(L) \\ m(\mu_1(L)) & m(\mu_2(L)) & \dots & m(\mu_n(L)) \end{pmatrix}, \tag{2.11.4}$$

where the eigenvalues of L are such that:

$$\mu_1(L) \leq \mu_2(L) \leq \ldots \leq \mu_n(L). \tag{2.11.5}$$

The eigenvalues of the Laplacian matrix L are bounded as

$$0 \leq \mu_j(L) \leq 2k_{max}, \tag{2.11.6}$$

and

$$\mu_n(L) \geq k_{max}. \tag{2.11.7}$$

The multiplicity of 0 as an eigenvalue of L is equal to the number of connected components in a network and the second smallest eigenvalue, $\mu_2(L)$, is commonly referred to as the algebraic connectivity of the network [23].

On the other hand, the normalised Laplacian matrix $\mathcal{L}$ is also positive semi-definite having eigenvalues

$$0 = \mu_1(\mathcal{L}) \leq \mu_2(\mathcal{L}) \leq \ldots \leq \mu_n(\mathcal{L}),$$

which are bounded [23] as

$$0 \leq \mu_j(\mathcal{L}) \leq 2, \tag{2.11.8}$$

and

$$\mu_n(\mathcal{L}) \geq \frac{n}{n-1}. \tag{2.11.9}$$

More on the spectrum of the normalised Laplacian $\mathcal{L}$ can be found in [41, 36]. The spectra of matrices A, L and $\mathcal{L}$ are related by the following inequalities [36]:

$$k_{max} - \mu_n(A) \leq \mu_n(L) \leq k_{max} - \mu_1(A), \tag{2.11.10}$$

and

$$\mu_j(\mathcal{L})k_{min} \leq \mu_j(\mathcal{L}) \leq \mu_j(\mathcal{L})k_{max}. \tag{2.11.11}$$

Some expressions for the spectra of different kinds of simple graphs are:

1. Path, $P_n : \mu_j(L) = 2 - 2\cos(\pi(j-1)/n)$, $j = 1, \ldots n$.
2. Cycle, $C_n : \mu_j(L) = 2 - 2\cos(2\pi j/n)$, $j = 1, \ldots n$.
3. Star, $S_n : Sp(L) = \{0,\, 1^{n-2}, n\}$.
4. Complete, $K_n : Sp(L) = \{0,\, n^{n-1}\}$.
5. Complete (bipartite), $K_{n_1,n_2} : Sp(L) = \{0,\, n_1^{n_2-1},\, n_2^{n_1-1}\}$.

Analysing the eigenvectors associated to the eigenvalues of L is also part of spectral graph theory. If we let Λ be a diagonal matrix of eigenvalues of the Laplacian matrix ordered as in the expression (2.11.5), then [36]

$$\Lambda = diag(\mu_1(L), \mu_2(L), \ldots, \mu_n(L)),$$

and let Φ be a matrix whose columns are orthonormal eigenvectors $\Phi_1, \Phi_2, \ldots, \Phi_n$.

Then the spectral decomposition of the Laplacian matrix is give by:

$$L = \Phi \Lambda \Phi^T.$$

The eigenvector of L associated with the 0 eigenvalue in a connected network is $\phi_1(L) = \frac{1}{\sqrt{n}}1$, and if $0 \neq \mu < n$ is an eigenvalue of the Laplacian, then the eigenvector associated with μ takes the value 0 on every node of degree $n-1$ [36]. The eigenvectors of the Laplacian contain useful information related to the structure of a network. The spectrum of this important matrix leads to the concept of algebraic connectivity of a network which is assigned to the eigenvalue μ_{n-1} , and the eigenvector associated with this value has an important property.

2.12 Summary

In this chapter, an introduction has been given to network theory at the level of providing the basic tools for reasoning about and analysing networked systems as they appear in this thesis. Specifically, an overview of the basic structures in network theory has been supplied, for example, definitions and types of networks. The structural properties of networks were then investigated. Moreover, some of the more important continuous probability distributions, for example, Normal and Cauchy distributions were considered. We then explored connections between graphs and their algebraic representation in terms of adjacency and Laplacian matrices, as well as the spectrum of the Laplacian graph and adjacency matrix.

Chapter 3

Dynamical Systems on Networks

3.1 Introduction

A system whose state, which is shown as a set of quantitative variables, changes over time in accordance with certain rules or equations, [86] is known as a dynamical system. Examples of dynamical systems are communication networks, and vehicles such as aircraft, spacecraft, motorcycles, or cars. Machines, robots, chemical plants, electrical circuits, even structures like bridges (think of a structure subject to strong winds or an earthquake) also qualify as dynamical systems. Apart from engineering systems, the concept of dynamical systems is applicable to plants, groups of animals, human beings or the economy a country or countries. Dynamical processes are the interactions among the parts that a network is comprised and can be considered on a continuous or discrete time basis.

A review of notions relating to dynamical systems is necessary at this juncture, since at a later point in this thesis dynamical processes on complex networks will be dealt with. Not everything in this field is going to be covered, but certain simple concepts related to this thesis in some way will be presented. There is an abundance of literature on the topic of dynamical systems – this chapter will merely scratch the surface.

3.2 Random walks and Lévy flights

In stochastic optimization, random walks comprise a significant part of the search process. However, the actual algorithm of interest may determine the exact form. Here the main concepts of random walks and Lévy flights, and their role in stochastic search are discussed.

3.2.1 Random Walks

A random walk is a random process consisting of taking a series of consecutive random steps [139]. Let S_N denote the sum of each consecutive random step X_i, then S_N forms a random walk.

$$S_N = \sum_{i=1}^{N} X_i = X_1 + X_2 + \ldots + X_N = \sum_{i=1}^{N-1} X_i + X_N = S_{N-1} + X_N,$$

where X_i is a random step drawn from a random distribution. This relationship can also be considered a recursive formula. That is, the next state S_N will only depend on the current existing state S_{N-1} and the motion or transition X_N from the existing state to the next state, which typically constitutes the main property of a Markov chain. Here, the step size or length in a random walk can be fixed or it can vary.

A random walk is a stochastic process in which particles or waves travel along random trajectories. The first application of a random walk was in the description of particle motion in a fluid (Brownian motion). Now it is a central concept in statistical physics, describing transport phenomena such as heat, sound and light diffusion, as well as in many applications, such as economics, computer sciences, environmental science and engineering.

Mathematically speaking, a random walk is represented in the following equation;

$$S_{t+1} = S_t + w_t,$$

where S_t is the current location or state at t , and w_t is a step or random variable with a known distribution. If each step or jump is carried out in the d-dimensional space, the random walk S_N discussed earlier evolves into a random walk in higher dimensions. Additionally, there is no reason why each step length should be fixed. Essentially, the step size can also vary according to a known distribution. If the step length obeys the Gaussian distribution, the random walk becomes the Brownian motion or a diffusion process.

In theory, as the number of steps N increases, the central limit theorem implies that the random walk should approach a Gaussian distribution. As the mean of particle locations is zero, their variance will increase linearly with t. In general, in the d-dimensional space, the variance of Brownian random walks can be written as;

$$\sigma^2(t) =\mid v_0 \mid^2 t^2 + (2dD)t, \tag{3.2.1}$$

where v_0 is the drift velocity of the system. Here $D = s^2/(2\tau)$ is the effective diffusion coefficient, related to the step length s over a short time interval τ during each jump.

Therefore, the Brownian motion $B(t)$ essentially obeys a Gaussian distribution with zero mean and time-dependent variance. That is, $B(t) \sim N(0, \sigma^2(t))$ where $\sim$ means that the random variance obeys the distribution on the right-hand side; that is, samples should be drawn from the distribution. A diffusion process can be viewed as a series of Brownian motions, obeying the Gaussian distribution. For this reason, standard diffusion is often referred to as Gaussian diffusion. If the motion at each step is not Gaussian, then the diffusion is called non-Gaussian diffusion.

If the step lengths obey other distributions, we have to deal with more generalised random walks. In particular, when step lengths obey the Lévy distribution, such a random walk is termed a Lévy flight or a Lévy walk.

3.2.2 Lévy flights

Lévy flights are Markovian stochastic processes whose individual jumps have lengths that are distributed with a probability density function (PDF) $p(x)$ decaying at large x as

$$p(x) \sim \mid x \mid^{-1-\alpha},$$

with $0 < \alpha \leq 2$. Due to their divergent variance, $< x^2(t) > \longrightarrow \infty$, rather long jumps may occur, and typical trajectories are self-similar, on all scales, characterised by clusters of shorter jumps interspersed with long excursions. Similar to the emergence of the Gaussian as a limit distribution of independent identically distributed (iid) random variables with finite variance due to the central limit theorem, Lévy stable distributions represent the limit distributions of (iid) random variables with diverging variance. In that sense, the limiting case of the basin of attraction of the so-called generalised central limit theorem for $\alpha = 2$ [64] is represented by the Gaussian distibution.

Mathematically speaking, a definition of Lévy distribution should be rendered in terms of the following Fourier transform:

$$\mathcal{F}(k) = \exp(-\beta \mid k \mid^{\alpha}),\ 0 < \alpha \leq 2, \tag{3.2.2}$$

where β is a scale parameter. The inverse of this integral is not easy, as it does not have analytical form, except for a few special cases. The special case $\alpha = 2$ corresponds to a Gaussian distribution, while $\alpha = 1$ leads to a Cauchy distribution. For the general case, the inverse integral

$$p(x) = \frac{1}{\pi} \int_0^{\infty} \cos(kx) \exp(-\beta \mid k \mid^{\alpha}) dk, \tag{3.2.3}$$

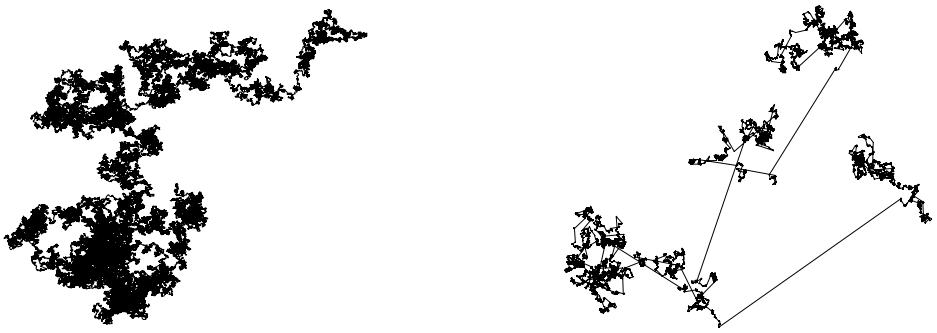


Figure 3.2.1: Comparison of the trajectories of a Gaussian (left) and a Lévy (right) processes, the latter with index $\alpha = 1.5$.

can be estimated only when x is large. We have

$$p(x) \sim \frac{\alpha\beta\Gamma(\alpha)\sin(\pi\alpha/2)}{\pi \mid x \mid^{1+\alpha}},\ x \longrightarrow \infty. \tag{3.2.4}$$

Here $\Gamma(z)$ is the Gamma function

$$\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}dt. \tag{3.2.5}$$

If $z = n$ is an integer, we have $\Gamma(n) = (n-1)!$.

Lévy flights demonstrate greater efficiency than Brownian random walks when unknown, large-scale search space is being investigated. Such efficiency can be explained in many ways: one of them being the fact that there is a much more rapid increase in the variance of Lévy flights than in the linear relationship (i.e., $\sigma^2(t) \sim t$) of Brownian random walks.

$$\sigma^2(t) \sim t^{3-\alpha},\ 1 \leq \alpha \leq 2, \tag{3.2.6}$$

A significant point worth mentioning relates to the link between a power-law distribution and some scale-free characteristics. In this way self-similarity and fractal behaviour can be observed in Lévy flight patterns.

3.3 Dynamical Systems

A dynamical system can be defined as a triple $\mathbb{S} = (\mathbb{T}, \mathbb{W}, \mathfrak{V})$, where $\mathbb{T}$ is a subset of $\mathbb{R}$, i.e. the time axis, $\mathbb{W}$ is a set known as the signal space, and $\mathfrak{V}$ is a subset of $\mathbb{W}^{\mathbb{T}}$ called the behaviour[1] [100]. The set $\mathbb{T}$ states the set of times instances relating to our problem, and usually equals $\mathbb{R}$ or $\mathbb{R}_+$ in continuous-time systems, and $\mathbb{Z}$ or $\mathbb{Z}_+$ in discrete-time systems. The set $\mathbb{W}$ defines the formalisation of the outcomes of the signals produced by the dynamical system as elements of a set, that is, these outcomes are the variables whose evolution in time is being described [100]. Behaviour $\mathfrak{V}$ is a family of time trajectories that take their values in the signal space, that is to say, the elements of $\mathfrak{V}$ are the trajectories compatible with the laws that govern the system. In most models equations are used to describe the behaviour, and then those elements satisfying a set of equations which often take the form of differential equations for continuous-time models, and difference equations for discrete-time models, form this set.

There are two types of dynamical systems, continuous and discrete-time ones and they can be either deterministic or stochastic.

3.3.1 Continuous dynamical systems

A continuous dynamical system described by a single real variable $y(t)$ that evolves according to a first-order differential equation is

$$y'(t) = f(y(t));\ y(0) = y_0, \tag{3.3.1}$$

where $f(y(t))$ is some specified function of $y(t)$. Frequently, there is an initial condition that specifies the value of variable y at some initial time t_0, and is expressed as y_0. A deterministic dynamical system is one in which the equations that describe the evolution of time are continuous functions.

[1] $\mathbb{W}^{\mathbb{T}}$ is standard mathematical notation for the collection of maps from $\mathbb{T}$ to $\mathbb{W}$ [100].

3.3.2 Discrete dynamical systems

The concept of discreteness is directly related to the concept of discrete time, i.e. we suppose that we measure time in discrete units, which might be hours, seconds, years, centuries or any other period of time of which, once fixed, only integer multiples may be considered. We represent the state of a system at time $t = 0$ by $y(0)$ and the state of the system at the k-th time step as $y(k)$. A discrete dynamical system is a system in which the state at any time depends only on the state a the time before [94], then discrete dynamical systems are specified by the equations:

$$y(t+1) = f(y(t));\ y(0) = y_0. \tag{3.3.2}$$

The dynamic system (3.3.2) is often called a difference equation. It follows that $y(t) = f^n(y_0)$, where $f^n = f \circ f \circ f \ldots \circ f$ is the k-fold application of f to y_0.

3.4 Stochastic process

Definition 3.1. A stochastic process is a family of random variables denoted as $\{X(t),\, t \geq 0\}$, where t is a parameter running over a suitable index set T.

Stochastic processes for which $T = [0, \infty)$ are particularly important for applications. There are two particularly important types of processes, Poisson processes and Markov processes.

Definition 3.2. A Poisson process with parameter or rate $\lambda > 0$ is an integer-valued, continuous time stochastic process $\{X(t),\, t \geq 0\}$ satisfying

- $X(0) = 0$.
- For all $t_0 = 0 < t_1 < t_2 < \ldots < t_n$, the increments $X(t_1) - X(t_0)$, $X(t_2) - X(t_1), \ldots, X(t_n) - X(t_{n-1})$ are independent random variables.
- For $t \geq 0$, $s > 0$ and non-negative integers k, the increments have a Poisson

distribution

$$\mathbb{P}(X(t+s) - X(s) = k) = \frac{(\lambda t)^k e^{-\lambda t}}{k!}.$$

Definition 3.3. A Markov process $\{X(t),\, t \in T\}$, is a stochastic process with the property that, given the value of $X(t)$, the values of $X(s)$, $s \in T$ and $s > t$ are not influenced by values of $X(u)$ with $u \in T$ and $u < t$. If the sample space is discrete, the Markov process is called Markov chain.

3.5 Dynamical processes on networks

It is possible to represent a number of real world phenomena as dynamical systems on networks. Examples would be the spread of information among a group of people, the movement of money in a country's economy, traffic on the roads, the flow of electricity over the grid, the evolution of population in an ecosystem, among other situations [86]. A considerable amount of attention has been given recently to the study of dynamical processes on networks due to the fact that many physical and engineering systems can be represented as networks of interacting entities [9, 36]. A ubiquitous physical process in most complex systems is diffusion. It is a fundamental process in any living organism, ranging from the transport of biomolecules to cell membranes to the specific interactions of proteins with DNA [108, 107, 11, 101, 65], in many social phenomena [111, 127], as well as in man-made systems [92].

Two principal approaches are utilised when dealing with dynamical processes on networks [9]. The first approach includes the identification of each node of the network with a single individual or element of the system, and in the second approach, we consider dynamical entities such as people, information packets, energy or matter flowing through a network whose nodes identify locations where the dynamical entities transit. In both approaches, the dynamical description of the system can be achieved by introducing a corresponding variable x_i that

characterises the dynamical state for each node i. Then, if each node represents a single individual, the variable x_i may describe a particular attribute of the individual.

In the case of dynamical entities moving in a network, the state variable x_i generally depends on the entities present at that node. All possible states $x_i = 1, 2, \ldots, k$ can be enumerated for each node and the knowledge of the state variable of all nodes in the network defines the (microscopic) state of the system [9]. Thus, a particular configuration of the network at time t by the set $x(t) = (x_1(t), (x_2(t), \ldots, (x_n(t))$ can be denoted, where n representing the number of nodes in the network. When referring to dynamics on networks, having independent dynamical variables on each node is commonly considered, coupled together along the edges of the network, that is, when writing an equation for the time evolution of a variable x_i the individual terms appearing in that equation involve x_i, other variables on vertex i, or one or more variables on a vertex adjacent to i in the network [86]. In real systems, adding the dimension of dynamics to the characterisation of networks facilitates a better comprehension of the systems being analysed through considering the interplay between structural and dynamical aspects [15].

3.6 A simple dynamical system on a network

If we assume that we have independent dynamical variables $x_i, y_i, \ldots,$ on each vertex i and that they are coupled together only along the edges of the network, equations describing the time evolution of the variables will involve only the variables themselves and other variables on vertex i or more variables on neighbours of vertex i. No term involving variables on non-nearest neighbours exists. Similarly, there is no term involving more than one adjacent vertex. For instance, let us consider the dynamic describing the time evolution of the probability of

infection of a vertex in a network of the type (continuous version):

$$\frac{dx_i}{dt} = \beta(1 - x_i) \sum_j A_{ij} x_i. \tag{3.6.1}$$

The dynamic described by this equation only involves pairs of variables that are connected by edges since these are the only pairs for which A_{ij} is non-zero. In general, for systems with a single variable on each vertex we have the equation [86]:

$$\frac{dx_i}{dt} = f_i(x_i) + \sum_j A_{ij} g_{ij}(x_i, x_j), \tag{3.6.2}$$

where the first term only involves variables on vertices and the second term involves variables on adjacent vertices. The function f_i describes how vertex i will evolve independently without the other vertices and g_{ij} describes only the contribution from the nearest connections themselves. The function g_{ij} also represents the coupling between variables on different vertices that are directly connected by an edge. The dynamic of each vertex is often the same and we can simply write,

$$\frac{dx_i}{dt} = f(x_i) + \sum_j A_{ij} g(x_i, x_j). \tag{3.6.3}$$

We also assume that the network is undirected such that if x_i is affected by x_j then x_j is similarly affected by x_i.

3.7 The Diffusion Process

In this section an example illustrating dynamical processes on a network is presented. In addition to the diffusion process, there are a number of other processes that can evolve on a network, such as consensus [9], epidemic spreading [9], or synchronisation [9]. We simply consider here the case of the diffusion process [86].

The process by which gas moves from regions of high density to regions of

low density is known as diffusion, and is driven by the radiative pressure or partial pressure of the different regions. We can consider on the other hand diffusion processes on networks and some times those processes are convenient simple models of spread across a network, such as the spread of an idea, or the spread of disease or any kind of information. Suppose we have some kind of substance on the vertices of a network and let ω_i be the amount of that substance on vertex i. Let us suppose that the substance moves along the edges, flowing from one vertex j to an adjacent vertex i at a rate $C(\omega_j - \omega_i)$ where C is a constant called the diffusion constant, i.e., in a short span of time the amount of fluid flowing from j to i is $C(\omega_j - \omega_i)dt$. The evolution equation of ω_i on the network is given by:

$$\frac{d\omega_i}{dt} = C\sum_j A_{ij}(\omega_j - \omega_i). \tag{3.7.1}$$

The adjacency matrix in this expression ensures that the only terms appearing in the sum are those that correspond to vertex pairs that are actually connected by an edge. In the case of an undirected network we can write the equation (3.7.1) as follows:

$$\begin{aligned}\frac{d\omega_i}{dt} &= C\sum_j A_{ij}\omega_j - C\omega_i\sum_j A_{ij} \\ &= C\sum_j A_{ij}\omega_j - C\omega_i k_i \\ &= C\sum_j (A_{ij} - \delta_{ij}k_i)\omega_j, \end{aligned} \tag{3.7.2}$$

where k_i is the degree of vertex i and δ_{ij} is the Kronecker symbol. In matrix notation we have

$$\frac{d\omega}{dt} = C(A - K)\omega, \tag{3.7.3}$$

where A is the adjacency matrix of the network and K is the matrix with the vertex degrees along its diagonal and ω is a vector whose components are ω_i . By

the definition of the Laplacian of the previous chapter, equation (3.7.3) can be written as

$$\frac{d\omega}{dt} = -CL\omega, \tag{3.7.4}$$

where $L = K - A$. This equation has the same form as the ordinary diffusion equation for a gas where the the Laplacian operator ∇^2 has been replaced by the Laplacian matrix L which also occurs in many places such as random walks on networks, resistor networks, graph partitioning and network connectivity.

The Solution Equation (3.7.4) can be solved by writing the unknown vector ω as a linear combination of the eigenvectors of the Laplacian matrix L. That is,

$$\omega(t) = \sum_i \alpha_i u_i. \tag{3.7.5}$$

Putting together equations (3.7.3) and (3.7.5) we have the following:

$$\sum_i (\frac{d\alpha_i}{dt} + C\lambda_i\alpha_i)u_i = 0. \tag{3.7.6}$$

Multiplying both sides of equation (3.7.5) by u_j and taking into account that eigenvectors of the Laplacian matrix are orthogonal we get

$$\frac{d\alpha_i}{dt} + C\lambda_i\alpha_i = 0, \ \forall i, \tag{3.7.7}$$

which has the solution

$$\alpha_i(t) = \alpha_i(0)e^{C\lambda_i t}, \tag{3.7.8}$$

thus the solution to equation (3.7.3) is

$$\omega(t) = \sum_i \alpha_i(0)e^{C\lambda_i t}u_i. \tag{3.7.9}$$

3.8 Anomalous diffusive processes

Anomalous diffusion is a diffusion process with a non-linear relationship to time, in which the mean squared displacement (MSD),

$$<\mid r \mid^2 (t) > \sim t^{\alpha}.$$

Unlike typical diffusion, anomalous diffusion occurs when $\alpha \neq 1$. In this case, the Central Limit Theorem no longer applies and the variance grows slower or faster than linearly in time. If $\alpha < 1$, the kind of diffusion is known as sub-diffusion, and the probability distribution is non-Gaussian. If $\alpha > 1$, the diffusion is known as superdiffusion. Motions with $\alpha = 2$ are also known as ballistic, which commonly have constant velocity, like particles from a bomb, rather than diffusive, like dye spreading [43].

The distinction between normal and anomalous diffusion can be understood by examining the rate at which velocity correlation decrease to zero. If the velocity correlation decreases rapidly, normal diffusion occurs. However, anomalous diffusion results from processes in which particles move coherently for long times with infrequent changes of direction. Generally speaking, this distinction is quantified by the tail behaviour of the velocity autocorrelation function. For example, if the correlation function decays exponentially, there is normal diffusion, whereas if the correlation function decays algebraically then anomalous diffusion is possible.

Modelling anomalous diffusion in the presence or absence of an external velocity or force field occur in a variety of ways, including fractional Brownian motion dating back to Benoît Mandelbrot, generalised diffusion equations, continuous time random walk models, Langevin equations, generalised Langevin equations, generalised master equations and generalised thermostatistics [79].

Over the last twenty years an impressive collection of literature has indicated that anomalous diffusion models exist. For example, anomalous diffusion is fre-

quently observed in materials with memory, for example, viscoelastic materials, and heterogeneous media, such as soil, heterogeneous aquifers, and underground fluid flow. At a microscopic level, the subdiffusion process can be described by a continuous time random walk, where the waiting time of particle jumps follows some heavy tailed distribution, whereas the superdiffusion process can be described by Lévy flights or Lévy walk, where the length of particle jumps follows some heavy tailed distribution, reflecting the long-range interactions among particles. If the aforementioned micro-macro correspondence is followed, the macroscopic counterpart of a continuous time random walk is a differential equation with a fractional derivative in time, and that for a Lévy flight is a differential equation with a fractional derivative in space [55].

3.9 The fractional diffusion equation (FDE)

The branch of mathematical analysis that deals with pseudo-differential operators that extend the standard notions of integrals and derivatives to any positive non-integer order is known as fractional calculus. In recent years the theory of fractional derivatives and integrals called fractional calculus has steadily increased in importance for diverse applications in various scientific and technological fields. Examples of these are a variety of many other physical processes [69, 99] such as thermal engineering, acoustics, electromagnetism, control systems, robotics, visco-elasticity, diffusion, edge detection, turbulence, and signal processing. Fractional differential equations FDEs have also been applied in modelling many physical engineering problems, as well as in fractional differential equations in non-linear dynamics [69]. Fractional derivatives and integrals of order $\alpha > 0$ are defined differently: Riemann-Liouville, Caputo, Grünwald-Letnikov, Weyl, Marchaud and Riesz [69, 99] because fractional operators take different kernel representations in different function spaces as a consequence of the non-local

character of fractional kernels [82]. In general, the Riemann–Liouville and the Caputo fractional operators [99] are two of the widely-used fractional operators. Both concern the so-called Riemann-Liouville fractional integral defined for any order $\alpha > 0$. The two definitions differ by reason of the order of evaluation.

However, the free motion of the particle was modelled by the classical diffusion equation

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u(x,t)}{\partial x^2},\ x \in \mathbb{R},\ t > 0, \tag{3.9.1}$$

where $u(x,t)$ represents the probability density function of finding a particle at the point x in the time instant t. Here D is a positive constant depending on the temperature, the friction coefficient, the universal gas constant and finally on the Avogadro number.

Assuming the external outside force acting towards the origin $x = 0$ and being proportional to the distance of the particle from the origin, equation (3.9.1) should be augmented by a drift term:

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial}{\partial x}(F(x)u(x,t)), \tag{3.9.2}$$

where $F(x)$ is the external force. Therefore, equation (3.9.2) can be interpreted as modelling the diffusion of a particle under the action of the external outside force $F(x)$.

Therefore, the fractional diffusion in time under external force, equation (3.9.2) becomes

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = D\frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial}{\partial x}(F(x)u(x,t)),\ 0 < \alpha \leq 1,\ D > 0, \tag{3.9.3}$$

where $\frac{\partial^\alpha}{\partial t^\alpha}$ are the Riemann-Liouville or Caputo derivatives of order a [103].

Definition 3.4. A real function $f(x)$, $x > 0$, is said to be in the space C_α, $\alpha \in \mathbb{R}$ if there exists a real number $p(> \alpha)$ such that $f(x) = x^p f_1(x)$, where $f_1(x) \in$

$C[0,\infty)$, and it is said to be in the space C_α^n if $f^{(n)} \in C_\alpha$, $n \in \mathbb{N}$.

Definition 3.5. The standard diffusion equation for the field $u(x,t)$ with initial condition $u(x,0+ = u_0(x)$ is

$$\frac{\partial u}{\partial t} = K_1 \frac{\partial^2 u}{\partial x^2},\ -\infty < x < \infty,\ t \geq 0,$$

where K_1 is a suitable diffusion coefficient of dimensions.

Definition 3.6. Riemann-Liouville fractional integration of order α is defined as

$$I^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_0^x (t-\tau)^{\alpha-1} f(\tau) d\tau,\ \alpha > 0,\ \tau > 0. \tag{3.9.4}$$

where Γ is the Gamma function defined in (3.2.5).

Definition 3.7. The fractional derivative of order $\alpha > 0$ in the Riemann-Liouville sense D_t^α is defined as

$$D^\alpha f(t) = \begin{cases} \frac{d^n}{dt^n}[\frac{1}{\Gamma(n-\alpha)} \int_\alpha^t (t-\tau)^{n-\alpha-1} f(\tau) d\tau & n-1 < \alpha < n \in \mathbb{N}, \\ \\ \frac{d^n}{dt^n} f(t) & \alpha = n \in \mathbb{N}. \end{cases}$$

Definition 3.8. the fractional derivative of order $\alpha > 0$ in the Caputo sense ${}_*D_t^\alpha$ is defined as

$${}_*D^\alpha f(t) = \begin{cases} \frac{1}{\Gamma(n-\alpha)} \int_\alpha^t (t-\tau)^{n-\alpha-1} f^{(n)}(\tau) d\tau & n-1 < \alpha < n \in \mathbb{N}, \\ \\ \frac{d^n}{dt^n} f(t) & \alpha = n \in \mathbb{N}. \end{cases}$$

One of the main advantages of the Caputo fractional derivative is that initial conditions are expressed in terms of initial values of integer order derivatives. As a consequence, the Caputo fractional derivative appears more suitable to be treated by the Laplace transform technique in that it requires the knowledge of the initial values of the function and of its integer order derivatives [24].

There are two distinct classes of partial differential equations that have a mixed character, i.e. that can be modelled both in continuous time as well as in discrete space

$$D_t v(n,t) = (-L)^{\alpha} v(n,t),\ t > 0,\ n \in \mathbb{Z}, \tag{3.9.5}$$

and

$$D_t^{1/\alpha} u(n,t) = (-L) u(n,t),\ t > 0,\ n \in \mathbb{Z}, \tag{3.9.6}$$

where D_t denotes the continuous derivative in the variable t and $D_t^{1/\alpha}$ denotes the fractional derivative of order $1/\alpha$ in the sense of Liouville (left-sided) and $(-L)$ denotes the fractional powers of order α of the unidimensional discrete Laplacian, introduced in [25]. For $\beta := \frac{1}{\alpha} > 1$, Eq. 3.9.6 describes superdiffusive phenomena in time. It models anomalous superdiffusion in which a particle cloud spreads faster than the classical diffusion model predicts. The connection between order in time and space for partial differential equations is a surprising phenomena that seems not to be addressed for the discrete fractional Laplacian [24]. it was proved that $\{e^{tL}\}_{t\geq 0}$ is a positive Markovian diffusion semigroup [25]. Moreover, for each $\varphi \in \ell^{\infty}(\mathbb{Z})$ the function $u(n,t) = e^{tL}\varphi(n)$ is a solution of the discrete heat equation, that is (3.9.5) with $\alpha = 1$.

3.10 Summary

The aim of this chapter was to briefly cover the dynamics on networks. We started by defining some basic concepts from graph theory which will be used through

this work. We have briefly defined what a dynamical system is, and we have showed some examples of the possible dynamics that can modelled on a network, such as normal and anomalous diffusion processes. Moreover, we provided some basic analysis and observations about random walks and Lévy flights. Finally we have considered the fractional differential equations and the two most commonly used definitions: the Riemann-Liouville and Caputo derivatives. All the theory presented can be studied more deeply by going into the references provided.

Chapter 4

The k-path Laplacian operators

4.1 Introduction

The introduction of the k-path LOs potentially helps with more precise studies of the structures of a network's dynamics corresponding to different applications. However, there also need for study of the main properties of the k-path LOs, as greater understanding of the properties of these operators can lead to advances in algebraic graph theory.

The main goal of the present chapter is to investigate different aspects of the k-path LOs, which, through their generalisation, can help study undirected, simple, connected and infinite but locally finite networks. This chapter describes adjoints, and studies domains of essential self-adjointness for a class of differential operators on undirected graphs. We intend to characterise the infinite networks for which the operator L_k still generates a strongly continuous operator semigroup or even an analytic semigroup, in order to investigate diffusion models (also discussed in the following chapter). Our task is to specifically tackle when the k-path Laplacian L_k is self-adjoint on an infinite graph and when it is bounded. Furthermore, the transformed k-path Laplacian operators using Laplace, Factorial and Mellin transforms will also be studied.

4.2 Generalised definition of k-path Laplacian operators on graphs

A new kind of graph-theoretic matrix that generalises the graph Laplacian on finite graph was introduced in [35]. These matrices are based on the path matrices that characterize the existence of shortest paths between pairs of nodes in a graph. To construct these kinds of matrices, we need to consider these definitions:

Definition 4.1. The irreducible set of shortest paths of length l is define as the set $P_l = \{P_l(v_i, v_j), P_l(v_i, v_r), \ldots, P_l(v_s, v_t)\}$ in which the endpoints of every shortest path $P_l(v_i, v_j)$ in the set are different. Every shortest-path in this set is called an irreducible shortest path.

Definition 4.2. A k-hopping walk of length l is any sequence of (not necessarily different) nodes $v_1, v_2, \cdots, v_l, v_{l+1}$ such that $d_{i,i+1} = k$ for each $i = 1, 2, \cdots l$. This k-hopping walk is referred to as a k-hopping walk from v_1 to v_{l+1}.

Obviously, this generalizes the concept of walk because a walk of length l is a 1-hopping walk of length l. If every node of a graph can be visited by a k-hopping walk we say that the graph is k-hopping connected or simply that it can be k-hopped. Obviously, the number of connected components in a graph is equal to its number of 1-hopping connected components.

Definition 4.3. A k-hopping connected component in a graph $G = (V, E)$ is a subgraph $G' = (V', E')$, such that there is at least one k-hopping walk that visits every node $v_i \in V'$.

Definition 4.4. The k-path degree $\delta_k(v_i)$ $(k \leq d_{max})$ of a node v_i is the number of irreducible shortest-paths of length k having v_i as an endpoint. It is evident that $\delta_1(v_i)$ is the 'classical' node degree, i.e., the number of edges incident to v_i.

Then, the generalized Laplacian matrix on finite graph is defined as follows:

Definition 4.5. The k-path Laplacian matrix $L_k(k \leq d_{max})$ of a connected undirected graph $G = (V, E)$ is defined as the square symmetric $n \times n$ matrix whose entries are given by:

$$L_k(i, j) = \begin{cases} -1 & d_{ij} = k, \\ \delta_k(i) & i = j, \\ 0 & otherwise. \end{cases} \tag{4.2.1}$$

It is evident that $L_1 = L$ is the so-called Laplacian matrix of a graph, i.e., $L_1 = L = K - A$.

Example. Consider the k-path Laplacian operators of the graph illustrated in Fig. 4.2.1.

$$L_1 = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & -1 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & -1 & 0 & -1 & 2 \end{bmatrix}, \qquad L_2 = \begin{bmatrix} 2 & 0 & -1 & 0 & -1 \\ 0 & 1 & 0 & -1 & 0 \\ -1 & 0 & 2 & 0 & -1 \\ 0 & -1 & 0 & 1 & 0 \\ -1 & 0 & -1 & 0 & 2 \end{bmatrix},$$

$$L_3 = \begin{bmatrix} 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Definition 4.6. The k-path incidence matrix ($k \leq d_{max}$), denoted by B_k, of a connected graph of n nodes and p irreducible shortest paths of length k, is a matrix of p rows and n columns in which the rows correspond to the elements of

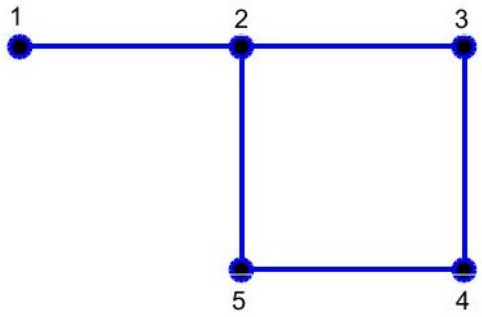


Figure 4.2.1: Example of simple graph.

the irreducible set of shortest-paths in the graph in which the paths are arbitrarily oriented from head to tail and the columns correspond to the nodes of the graph, $v_1, v_2, \cdots, v_n$. Then, the (i, j) entry of B_k is defined as:

$$B_k(i, j) = \begin{cases} +1 \quad if \quad v_j \text{ is the head of the irreducible shortest path } p_i, \\ -1 \quad if \quad v_j \text{ is the tail of the irreducible shortest path } p_i, \\ 0 \qquad \text{otherwise.} \end{cases} \tag{4.2.2}$$

Definition 4.7. A quadratic form is an expression of the form $q(x) = x^T Ax$, where x is a column vector and A is a symmetric matrix [10].

A quadratic form q is positive definite if $q(x) > 0$, and positive semi-definite if $q(x) \geq 0$, for every non-zero vector x.

Definition 4.8. The k-path matrix ($k \leq d_{max}$), denoted by P_k, of a connected graph of n nodes is the square, symmetric, $n \times n$ matrix whose entries are defined

as follows:

$$P_k(i,\, j) = \begin{cases} 1 & d_{i,j} = k, \\ 0 & \text{otherwise.} \end{cases} \tag{4.2.3}$$

Notice that $\delta_k(v_i) = (1^T P_k)_i$, where 1 is an all-ones column vector. It can be seen that the quadratic form is an expression of the form

$$y^T L_k y = \frac{1}{2} \sum_{i,j \in P_k(v_i, v_j)} (y_i - y_j)^2, \tag{4.2.4}$$

for any column vector y. As a consequence, the k-path Laplacian matrices L_k are positive semi-definite.

Moreover the k-path Laplacian for finite graph can be written also in the form;

$$(L_k\, f)(p) = \sum_{q:dist(p,q)=k} (f(p) - f(q)), \tag{4.2.5}$$

where dist denotes the shortest paths distance in G. Note that L_k is symmetric and bounded [35]. For infinite graphs the self-adjointness and also the boundedness depends on properties of the networks; this dependence will be studied for various classes of infinite networks.

In the following we always consider $G = (V,\, E)$ to be an undirected, locally finite (i.e. every node has a finite degree) and connected infinite graph with set of vertices V and set of edges E. Let d be the distance metric on G, i.e. $d(v,\, w)$ is the length of the shortest path from v to w, and let $\delta_k(v)$ be the k-path degree of the vertex v, i.e.

$$\delta_k(v) := \#\{w \in V :\, d(v, w) = k\}. \tag{4.2.6}$$

Since G is locally finite, $\delta_k(v)$ is finite for every $v \in V$. Denote by $C(V)$ the set of all complex-valued functions on V and by $C_0(V)$ the set of complex-valued

functions on V with finite support. Moreover, let $\ell^2(V)$ be the Hilbert space of square-summable functions on V with inner product

$$\langle f,\, g\rangle = \sum_{v\in V} f(v)\overline{g(v)}, \qquad f, g \in \ell^2(V). \tag{4.2.7}$$

In $\ell^2(V)$ there is a standard orthonormal basis consisting of the vectors e_v, $v \in V$, where

$$e_v(w) := \begin{cases} 1 & \text{if } w = v, \\ 0 & \text{otherwise.} \end{cases} \tag{4.2.8}$$

Let $\mathcal{L}_k$ be the following mapping from $C(V)$ into itself:

$$\big(\mathcal{L}_k\, f\big)(v) := \sum_{w\in V:\, d(v,w)=k} \big(f(v) - f(w)\big), \qquad f \in C(V). \tag{4.2.9}$$

On the vectors e_v it acts as follows:

$$(\mathcal{L}_k\, e_v)(w) = \begin{cases} \delta_k(v) & \text{if } \ w = v, \\ -1 & \text{if } \ d(v,w) = k, \\ 0 & \text{otherwise.} \end{cases} \tag{4.2.10}$$

We define $L_{k,min}$ and $L_{k,max}$, the *minimal and maximal k-path Laplacians*, as the restrictions of $\mathcal{L}_k$ to

$$\mathrm{dom}(L_{k,min}) = C_0(V) \qquad \text{and} \qquad \mathrm{dom}(L_{k,max}) = \big\{f \in \ell^2(V) : \mathcal{L}_k f \in \ell^2(V)\big\},$$

respectively. Clearly, $e_v \in \mathrm{dom}(L_{k,min})$, and we obtain from (4.2.10) that

$$\|L_{k,min}e_v\| = \sqrt{\big(\delta_k(v)\big)^2 + \delta_k(v)} = \begin{cases} 0 & \text{if } \delta_k(v) = 0, \\ \\ \delta_k(v)\sqrt{1 + \frac{1}{\delta_k(v)}} & \text{if } \delta_k(v) > 0. \end{cases} \tag{4.2.11}$$

Proposition 4.9. *Suppose that $L_{k,min}$ and $L_{k,max}$ are defined as above; then*

$$L^*_{k,min} = L_{k,max}, \tag{4.2.12}$$

where $L^*_{k,min}$ represents the adjoint of the k-path Laplacian operators $L_{k,min}$.

Proof. Let $f \in C_0(V)$ and $g \in C(V)$, let V_{00} be the support of f and set

$$V_0 := V_{00} \cup \big\{v \in V : \exists\, w \in V_{00} \text{ such that } d(v,w) = k\big\}, \tag{4.2.13}$$

which is a finite set because the graph is a locally finite and V_{00} is a finite set. Then $\operatorname{supp} \mathcal{L}_k f \subset V_0$ and the following relation holds:

$$\sum_{v\in V}(\mathcal{L}_k\, f)(v)\,\overline{g(v)} = \sum_{v\in V_0}(\mathcal{L}_k\, f)(v)\,\overline{g(v)} = \sum_{\substack{v,w\in V_0:\\ d(v,w)=k}} \big(f(v) - f(w)\big)\,\overline{g(v)}$$

$$= \frac{1}{2}\left[\sum_{\substack{v,w\in V_0:\\ d(v,w)=k}} \big(f(v) - f(w)\big)\,\overline{g(v)} + \sum_{\substack{v,w\in V_0:\\ d(v,w)=k}} \big(f(w) - f(v)\big)\,\overline{g(w)}\right] \tag{4.2.14}$$

$$= \frac{1}{2} \sum_{\substack{v,w\in V_0:\\ d(v,w)=k}} \big(f(v) - f(w)\big)\,\overline{(g(v) - g(w))} \tag{4.2.15}$$

$$= \frac{1}{2} \left[\sum_{\substack{v,w\in V_0:\\ d(v,w)=k}} f(v)\,\overline{(g(v) - g(w))} + \sum_{\substack{v,w\in V_0:\\ d(v,w)=k}} f(w)\,\overline{(g(w - g(v))} \right] \tag{4.2.16}$$

$$= \sum_{\substack{v,w\in V_0:\\ d(v,w)=k}} f(v)\,\overline{(g(v) - g(w))} = \sum_{v\in V_{00}} f(v)\,\overline{(\mathcal{L}_k\, g)(v)} \tag{4.2.17}$$

$$= \sum_{v\in V} f(v)\,\overline{(\mathcal{L}_k\, g)(v)}. \tag{4.2.18}$$

Let $g \in \mathrm{dom}(L_{k,max})$. It follows from (4.2.18) that

$$\langle L_{k,min}\, f,\, g\rangle = \langle f,\, L_{k,max}\, g\rangle,$$

for all $f \in \mathrm{dom}(L_{k,min})$, which implies that $g \in \mathrm{dom}(L^*_{k,min})$. Now let $g \in \mathrm{dom}(L^*_{k,min})$. For each $v \in V$ we obtain from (4.2.18) with $f = e_v$ that

$$\overline{(L^*_{k,min}\, g)(v)} = \langle e_v,\, L^*_{k,min}\, g\rangle = \langle L_{k,min}\, e_v,\, g\rangle = \sum_{w\in V} (\mathcal{L}_k\, e_v)(w)\,\overline{g(w)}$$

$$= \sum_{w\in V} e_v(w)\,\overline{(\mathcal{L}_k\, g)(w)} = \overline{(\mathcal{L}_k g)(v)},$$

which implies that $L^*_{k,min} g = \mathcal{L}_k g$. Since $L^*_{k,min} g \in \ell^2(V)$ by the definition of the adjoint, it follows that $g \in \mathrm{dom}(L_{k,max})$. Hence $L^*_{k,min} = L_{k,max}$. □

Since $L_{k,max}$ is an extension of $L_{k,min}$, it follows that $L_{k,min}$ is a symmetric operator. Moreover, for $f = g$ we obtain from (4.2.15) that

$$\big\langle L_{k,min}\, f,\, f\big\rangle = \frac{1}{2} \sum_{\substack{v,w\in V_0:\\ d(v,w)=k}} \big|f(v) - f(w)\big|^2, \tag{4.2.19}$$

where V_0 is as in (4.2.13); this shows that $L_{k,min}$ is a non-negative operator.

Also, if a subset V_0 of V ($V_0 \subset V$) is a k-hopping component, then $C(V_0)$ considered as a subspace of $C(V)$ is $\mathcal{L}_k$-invariant.

Lemma 4.10. *Let V_0 be a k-connected component of V and let $f \in C(V_0)$ be real-valued and bounded such that f attains its supremum. If*

$$\big(\mathcal{L}_k f\big)(v) \leq 0 \quad \textit{for every } v \in V_0, \tag{4.2.20}$$

then f is constant on V_0.

Proof. Assume that f is not constant. Then there exist v_0, $v_1 \in V_0$ such that

$$f(v_0) = \max\{f(v) : v \in V_0\},$$

$$f(v_1) < f(v_0), \qquad d(v_1, v_0) = k.$$

This implies that

$$\big(\mathcal{L}_k f\big)(v_0) = f(v_0) - f(v_1) + \sum_{\substack{w \neq v_1: \\ d(w,v_0)=k}} \big(f(v_0) - f(w)\big) > 0,$$

which is a contradiction to (4.2.20). Hence f is constant on V_0. □

Next we show that $L_{k,min}$ is actually essentially self-adjoint; see, e.g. [57, 135, 138] for the case $k = 1$.

Theorem 4.11. *The operator $L_{k,min}$ is essentially self-adjoint and hence $L_{k,max}$ is self-adjoint and it is equal to the closure of $L_{k,min}$.*

Proof. Since $L_{k,min}$ is non-negative and $L_{k,min}^* = L_{k,max}$, then by Proposition 1.41 it just needs to show that -1 is not an eigenvalue of $L_{k,max}$. Assume that this is not the case. Then there exists an $f \in \ell^2(V)$ such that $f \not\equiv 0$ and $L_{k,max} f = -f$. The function f must be zero on every finite k-hopping component since $L_{k,max}$ restricted to such a component is self-adjoint and non-negative. Therefore there

exists an infinite k-hopping component V_0 where f is not identically zero. It follows that

$$\delta_k(v)\, f(v) - \sum_{w:\, d(v,w)=k} f(w) = -f(v),$$

for $v \in V_0$, or equivalently,

$$\big(\delta_k(v)+1\big)\, f(v) = \sum_{w:\, d(v,w)=k} f(w).$$

Taking the modulus on both sides we obtain

$$\big(\delta_k(v)+1\big)\, |f(v)| \le \sum_{w:\, d(v,w)=k} |f(w)|.$$

Now we consider the function $|f|$:

$$\big(\mathcal{L}_k|f|\big)(v) = \delta_k(v)\, |f(v)| - \sum_{w:\, d(v,w)=k} |f(w)| \le -|f(v)| \le 0.$$

Since $f|_{V_0} \in \ell^2(V_0)$, the function $|f|$ attains the supremum on V_0. Hence Lemma 4.10 yields that $|f|$ is constant on V_0. This implies that $f = 0$ on V_0 because V_0 is infinite; a contradiction. □

We denote the closure of $L_{k,min}$ by L_k and call it the *k-path Laplacian*. By the previous theorem we have $L_k = L_{k,max}$; it is a self-adjoint and non-negative operator in $\ell^2(V)$. Note the difference in notation between the mapping $\mathcal{L}_k$ acting in $C(V)$ and the self-adjoint operator L_k in $\ell^2(V)$.

We can now estimate quadratic forms: for $f \in \mathrm{dom}(L_{k,min}) = C_0(V)$ we obtain from (4.2.19) that

$$\big\langle L_{k,min} f,\, f\big\rangle = \frac{1}{2} \sum_{\substack{v,w\in V:\\ d(v,w)=k}} \big|f(v)-f(w)\big|^2 \le \frac{1}{2} \sum_{\substack{v,w\in V:\\ d(v,w)=k}} \Big(|f(v)|+|f(w)|\Big)^2 \quad (4.2.21)$$

$$\leq \sum_{\substack{v,w\in V:\\ d(v,w)=k}} \Big(|f(v)|^2 + |f(w)|^2 \Big) \tag{4.2.22}$$

$$= \sum_{v\in V} \delta_k(v)\, |f(v)|^2 + \sum_{w\in V} \delta_k(w)\, |f(w)|^2 \tag{4.2.23}$$

$$= 2 \sum_{v\in V} \delta_k(v)\, |f(v)|^2. \tag{4.2.24}$$

In the next theorem we answer the question when L_k is a bounded operator.

Theorem 4.12. *The operator L_k is bounded if and only if δ_k is a bounded function on V. Now assume that δ_k is bounded and set*

$$\delta_{k,max} := \{\delta_k(v) : v \in V\}; \tag{4.2.25}$$

then

$$\delta_{k,max} \leq \|L_k\| \leq 2\delta_{k,max}. \tag{4.2.26}$$

Proof. If δ_k is unbounded, we choose a sequence $(v_i)_{i\in\mathbb{N}}$ in V with $sup_{i\in\mathbb{N}}\delta_k(v_i) = \infty$ and define $f_i : V \to \mathbb{C}$ by $f_i(v_i) = 1$ and $f_i(w) = 0$ if $w \neq v_i$, $w \in V$. Then we have $f_i \in \mathrm{dom}(L_{k,max})$ and

$$(L_k\, f_i)(w) = \begin{cases} -1 & \text{if } d(v_i, w) = k, \\ \delta_k(v_i) & \text{if } w = v_i, \\ 0 & \text{otherwise.} \end{cases}$$

Hence, $\| L_k f_i \|^2 = \delta_k(v_i)^2 + \delta_k(v_i)$ is unbounded but $\| f_i \| = 1$. Then (4.2.11) immediately shows that L_k is unbounded. Now assume that δ_k is bounded. Relation (4.2.11) yields the lower bound for $\|L_k\|$ in (4.2.26). From (4.2.24) we obtain

that for $f \in \mathrm{dom}(L_{k,min})$,

$$\left\langle L_{k,min}\, f,\, f \right\rangle \leq 2\delta_{k,max} \sum_{v \in V} |f(v)|^2 = 2\delta_{k,max} \|f\|^2.$$

Since L_k is self-adjoint and L_k is the closure of $L_{k,min}$, this shows that L_k is bounded and that $\|L_k\| \leq 2\delta_{k,max}$. □

4.3 The transformed k-path Laplacian operators

In this section, we introduce modulations, or linear transformations of the k-path Laplacian. The modulated operators produce diffusion of anomalous forms which usually occurs under particle-particle interactions (we will study this in the next chapter). The present modulated operators will be used as effective operators for anomalous diffusion. Here the transformations of k-path L_k are defined as combinations of the form

$$\sum_{k=1}^{\infty} c_k L_k, \tag{4.3.1}$$

with some non-negative coefficients $c_k \in \mathbb{C}$. This combination describes interactions with all nodes where different strengths are used for nodes at different distances. In general, one uses a sequence c_k that is decreasing in k.

If all L_k are bounded and

$$\sum_{k=1}^{\infty} |c_k| \, \|L_k\| < \infty, \tag{4.3.2}$$

then the series in (4.3.1) converges to a bounded operator on $\ell^2(V)$. If, in addition, $c_k \in \mathbb{R}$ for all $k \in \mathbb{N}$, then the operator in (4.3.1) is self-adjoint; if $c_k \geq 0$ for all $k \in \mathbb{N}$, then it is a non-negative operator.

Now, we study three different transformations of the $k-$path Laplacian op-

erators, namely, Laplace, factorial and Mellin, with the aim of using them in generalised diffusion models on networks. In the following theorem we discuss these transformed operators in more detail.

Theorem 4.13. *Assume that δ_1 is bounded on V and let $\delta_{1,max}$ be as in* (4.2.25).

(i) The *Laplace-transformed k-Laplacian*

$$\widetilde{L}_{L,\lambda} := \sum e^{-\lambda k} L_k, \tag{4.3.3}$$

is a bounded operator when $\lambda \in \mathbb{C}$ with $\Re\lambda > \ln \delta_{1,max}$. It is non-negative if $\lambda \in (\ln \delta_{1,max}, \infty)$.

(ii) The *factorial-transformed k-Laplacian*

$$\widetilde{L}_{F,z} := \sum_{k=1}^{\infty} \frac{z^k}{k!} L_k, \tag{4.3.4}$$

is a bounded operator for every $z \in \mathbb{C}$. It is self-adjoint if $z \in \mathbb{R}$ and non-negative if $z \geq 0$.

(iii) Assume that $\delta_{k,max}$ satisfies

$$\delta_{k,max} \leq Ck^{\alpha}, \tag{4.3.5}$$

for some $\alpha \geq 0$ and $C > 0$; then the *Mellin-transformed k-Laplacian*

$$\widetilde{L}_{M,s} := \sum_{k=1}^{\infty} \frac{1}{k^s} L_k, \tag{4.3.6}$$

is a bounded operator for $s \in \mathbb{C}$ with $\Re s > \alpha + 1$.

Under the assumption (4.3.5) the operator $\widetilde{L}_{L,\lambda}$ from (4.3.3) is bounded for every $\lambda \in \mathbb{C}$ with $\Re\lambda > 0$.

Proof. It follows easily that $\delta_{k,max} \leq \delta_{1,max}^k$ and hence

$$\|L_k\| \leq 2\delta_{1,max}^k,$$

for every $k \in \mathbb{N}$ by Theorem 4.12. Therefore the convergence condition (4.3.2) is satisfied in items (i) and (ii) for the specified λ and $z \in \mathbb{C}$.

For the Laplace-transformed k-Laplacian:

$$\sum e^{-\lambda k} L_k \Rightarrow \sum \mid e^{-\lambda k} \mid\mid L_k \mid\mid \leq 2 \sum_{k=0}^{\infty} (e^{-(\Re e \lambda)} \delta_{1,max})^k < \infty.$$

Hence it converges for $\Re e \lambda > \ln \delta_{1,max}$.

For the factorial-transformed k-Laplacian:

$$\sum_{k=1}^{\infty} \frac{z^k}{k!} L_k \Rightarrow \sum_{k=1}^{\infty} \frac{\mid z^k \mid}{k!} \parallel L_k \parallel \leq 2 \sum_{k=1}^{\infty} \frac{(\mid z \mid \delta_{1,max})^k}{k!} < \infty.$$

Hence it converges for every $z \in \mathbb{C}$.

For the *Mellin-transformed k-Laplacian,* we observe that under the condition (4.3.5) the operators L_k satisfy

$$\|L_k\| \leq 2Ck^{\alpha}.$$

Hence also in this case the condition (4.3.2) is satisfied for $\widetilde{L}_{M,s}$ with $\Re s > \alpha + 1$ and for $\widetilde{L}_{L,\lambda}$ with $\Re \lambda > 0$. □

If the graph is finite, then there is no restriction on the parameters needed, i.e. one can choose any $\lambda \in \mathbb{C}$ in (i) and any $s \in \mathbb{C}$ in (iii).

The growth condition (4.3.5) is fulfilled for several infinite graphs such as a linear path graph (or chain) for which $\delta_{k,max} = 2$ for every $k \in \mathbb{N}$, an infinite ladder for which $\delta_{k,max} = 4$, and for triangular, square and hexagonal lattices for which $\delta_{k,max} = gk$, with $g = 6, 4, 3$, respectively, among many others. In general, this growth condition can be applied to any infinite graph with bounded degree.

However, it is not fulfilled for Cayley trees for which $\delta_{k,\max} = r\,(r-1)^{k-1}$ where r is the degree of the non-pendant nodes.

Let us now consider the situation when the operators L_k may be unbounded. The closed quadratic form $\mathfrak{l}_k$ corresponding to L_k in the sense of [60] is given by

$$\mathfrak{l}_k[f] := \frac{1}{2} \sum_{\substack{v,w\in V:\\ d(v,w)=k}} \big|f(v) - f(w)\big|^2,$$

with domain

$$\mathrm{dom}(\mathfrak{l}_k) = \bigg\{ f \in \ell^2(V) : \sum_{\substack{v,w\in V:\\ d(v,w)=k}} \big|f(v) - f(w)\big|^2 < \infty \bigg\}.$$

Assume that $c_k \geq 0$, $k \in \mathbb{N}$. Then

$$\sum_{k=1}^{N} c_k \mathfrak{l}_k, \tag{4.3.7}$$

is an increasing sequence of densely defined, closed, non-negative quadratic forms (see [60, Theorem VI.1.31]). By [60, Theorem VIII.3.13a] the sequence in (4.3.7) converges to a closed non-negative quadratic form $\tilde{\mathfrak{l}}$ that is given by

$$\tilde{\mathfrak{l}}_k[f] = \sum_{k=1}^{\infty} c_k \mathfrak{l}_k[f] = \frac{1}{2} \sum_{k=1}^{\infty} c_k \sum_{\substack{v,w\in V:\\ d(v,w)=k}} \big|f(v) - f(w)\big|^2,$$

$$\mathrm{dom}(\tilde{\mathfrak{l}}_k) = \bigg\{ f \in \bigcap_{k=1}^{\infty} \mathrm{dom}(\mathfrak{l}_k) : \sum_{k=1}^{\infty} c_k \mathfrak{l}_k[f] < \infty \bigg\}.$$

Assume now that

$$\sum_{k=1}^{\infty} c_k \delta_k(v) < \infty, \tag{4.3.8}$$

for every $v \in V$. Since

$$\mathfrak{l}_k[e_v] = \langle L_k e_v,\, e_v \rangle = \delta_k(v),$$

by (4.2.10), condition (4.3.8) implies that $e_v \in \mathrm{dom}(\tilde{\mathfrak{l}})$ for every $v \in V$, and hence the form $\tilde{\mathfrak{l}}$ is densely defined. By [60, Theorem VI.2.1] there exists a self-adjoint non-negative operator $\tilde{L}$ that corresponds to $\tilde{\mathfrak{l}}$ in the sense that

$$\tilde{\mathfrak{l}}[f,\, g] = \big\langle \tilde{L}\, f,\, g \big\rangle,\ for\ f \in \mathrm{dom}\big(\tilde{L}\big),\ g \in \mathrm{dom}\big(\tilde{\mathfrak{l}}\big).$$

Moreover, [60, Theorem VIII.3.13a] implies that the partial sums $\sum_{k=1}^{N} c_k L_k$ converge in the strong resolvent sense to the operator $\tilde{L}$.

As an example consider a tree where each vertex in generation $n \in \mathbb{N}_0$ has $n+1$ children. It is easy to see that there are $n!$ vertices in generation n and that

$$\delta_k(v) \leq (n+k)!,$$

for each vertex v in generation n. For $z \in (0,1)$ condition (4.3.8) is satisfied for the factorial transform since

$$\sum_{k=1}^{\infty} \frac{z^k}{k!}\, \delta_k(v) \leq \sum_{k=1}^{\infty} \frac{z^k}{k!}\, (n+k)! < \infty,$$

by Ratio test for every vertex v in generation n. Hence $\widetilde{L}_{F,z}$ is a self-adjoint operator on this tree. If one includes linear chains of growing length between each generation, then $\delta_k(v)$ is growing more slowly and also other transformed k-path Laplacians are self-adjoint operators.

Assume that we are in the situation as above, i.e. that $c_k \geq 0$ and that condition (4.3.8) is satisfied. It is not difficult to see that the quadratic form $\tilde{\mathfrak{l}}$ is a Dirichlet form, i.e. it is closed and non-negative and it satisfies $\tilde{\mathfrak{l}}[Cf] \leq \tilde{\mathfrak{l}}[f]$ for every mapping $C : \mathbb{C} \to \mathbb{C}$ with $C(0) = 0$ and $|Cx - Cy| \leq |x - y|$. By the Beurling–Deny criteria the operator $-\tilde{L}$ generates an analytic, positivity-preserving semigroup of contractions; see, e.g. [105, Appendix 1 to Section XIII.12]. In the next chapters we consider a situation where all L_k are bounded operators and

(4.3.2) is satisfied. In this case we can write $(e^{-t\tilde{L}})_{t\geq 0}$ for the semigroup.

4.4 Summary

This chapter aims to extend the k-path Laplacian operators to infinite graphs and study a number of their properties such as self-adjointness and boundedness. The aim was to extend the definition of k-path Laplacian operators to locally finite infinite graphs. In other words, now there are path Laplacian operators in a Hilbert space, but further investigations and analysis are still needed. Consequently, some of the main properties of these operators, such as the essentially self-adjointness and the boundedness were studied. First, we proved analytically that these k-path LOs are symmetric and non-negative operators. Subsequently, we proved analytically that the k-path LOs are bounded under certain conditions. Then three different transformations of the k-path LOs were obtained: namely the Laplace, Factorial and Mellin transformations, which differ in the rate of convergence to zero of their coefficients. It was shown that all three transformed k-path LOs are, in general, bounded under certain assumptions. These results stimulated us to take further steps towards achieving the main goal of the research, which will be explained in the next chapter.

Chapter 5

One-dimensional diffusion processes on graph

5.1 Introduction

The definition and some of the major properties of the k-path LOs such as the essentially self-adjointness and the boundedness have already been presented in the previous chapter. It is well known that the application of the standard Laplacian L_1 can only hop the diffusive 'particle' from a node of the network to one of its neighbours whereas the application of the k-path Laplacian L_k hops the particle to sites at distance k. Further research is still necessary on certain interesting aspects, however, one of which is the study of a generalised diffusion equation on graphs. This study focusses on the use of k-path LOs and their transformations.

Therefore, our prime goal in this chapter is to generalise the diffusive equation for infinite path graph, with the purpose of obtaining an expression for the transformed k-path LOs to account for the diffusion in networks where combination long-range hops play an important role. The content of this chapter is drawn from our published work [38].

5.2 The k-path Laplacians on the infinite path graph

The study of diffusion on graphs is a well-established physico-mathematical theory based on the graph-theoretic version of the diffusion equation [67, 42]

$$\frac{d}{dt}u(t) = -Lu(t), \tag{5.2.1}$$

$$u(0) = u_0, \tag{5.2.2}$$

where L — the discrete Laplacian — is defined via the adjacency matrix A of the graph and the diagonal matrix of vertex degrees K as $L = K - A$ [77, 83, 85] We consider here the infinite path graph (or chain) P_∞, i.e. the graph whose vertices can be identified with $\mathbb{Z}$ and each pair of consecutive numbers is connected by a single edge. We now use index notation and write $u = (u_n)_{n\in\mathbb{Z}}$ for elements in $\ell^2(P_\infty)$. The k-path Laplacian acts as follows

$$(L_k u)_n = 2u_n - u_{n+k} - u_{n-k}, \qquad n \in \mathbb{Z},\ u = (u_\mu)_{\mu\in\mathbb{Z}} \in \ell^2(P_\infty).$$

It can also be identified with a double-infinite matrix whose entries are

$$(L_k)_{\mu\nu} = 2\delta_{\mu,\nu} - \delta_{\mu,\nu-k} - \delta_{\mu,\nu+k}, \qquad \mu,\nu \in \mathbb{Z}, \tag{5.2.3}$$

where δ denotes the Kronecker delta defined as

$$\delta_{i,j} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

In order to consider the diffusion of particles on the graph, we let e_0 be as in (4.2.8), i.e.

$$(e_0)_n = \delta_{n,0}, \tag{5.2.4}$$

which describes a profile that is concentrated at the origin. Under the application

of the standard combinatorial Laplacian L_1 the particle hops to the neighbouring sites ± 1, whereas under the application of the k-path Laplacian L_k the particle hops to the sites $\pm k$:

$$(L_k e_0)_n = 2\delta_{n,0} - \delta_{n,-k} - \delta_{n,+k}.$$

Since $\delta_{k,max} = 2$ for every $k \in \mathbb{N}$, the transformed k-Laplacians $\tilde{L}_{L,\lambda}$, $\tilde{L}_{F,z}$ and $\tilde{L}_{M,s}$ from (4.3.3), (4.3.4) and (4.3.6), respectively, are bounded operators for $\lambda \in \mathbb{C}$ with $\Re\lambda > 0$, for every $z \in \mathbb{C}$ and every $s \in \mathbb{C}$ with $\Re s > 1$. These operators are self-adjoint and non-negative if $\lambda \in (0, \infty)$, $z \in (0, \infty)$ and $s \in (1, \infty)$, respectively. In the following lemma we find explicit representations of these operators.

Lemma 5.1. *Let $\lambda \in \mathbb{C}$ with $\Re\lambda > 0$, $z \in \mathbb{C}$ and $s \in \mathbb{C}$ with $\Re s > 1$, and let $\tilde{L}_{L,\lambda}$, $\tilde{L}_{F,z}$, $\tilde{L}_{M,s}$ be as in* (4.3.3), (4.3.4) *and* (4.3.6), *respectively. Then for any $u \in \ell^2(P_\infty)$ we have*

$$\big(\tilde{L}_{L,\lambda}u\big)_n = \frac{2}{e^\lambda - 1}u_n - \sum_{k=1}^{\infty} e^{-\lambda k}\big(u_{n-k} + u_{n+k}\big),$$

$$\big(\tilde{L}_{F,z}u\big)_n = 2(e^z - 1)u_n - \sum_{k=1}^{\infty} \frac{z^k}{k!}\big(u_{n-k} + u_{n+k}\big),$$

$$\big(\tilde{L}_{M,s}u\big)_n = 2\zeta(s)u_n - \sum_{k=1}^{\infty} \frac{1}{k^s}\big(u_{n-k} + u_{n+k}\big),$$

where ζ is Riemann's zeta function defined in (1.8.2).

Applying them to e_0 we obtain

$$\left(\tilde{L}_{L,\lambda}e_0\right)_n = \begin{cases} \dfrac{2}{e^\lambda - 1} & \text{if } n = 0, \\ -e^{-\lambda|n|} & \text{if } n \neq 0, \end{cases} \qquad \left(\tilde{L}_{F,z}e_0\right)_n = \begin{cases} 2(e^z - 1) & \text{if } n = 0, \\ -\dfrac{z^{|n|}}{|n|!} & \text{if } n \neq 0, \end{cases} \tag{5.2.5}$$

$$\left(\tilde{L}_{M,s}e_0\right)_n = \begin{cases} 2\zeta(s) & \text{if } n = 0, \\ -\dfrac{1}{|n|^s} & \text{if } n \neq 0. \end{cases} \tag{5.2.6}$$

Proof. Let c_k, $k \in \mathbb{N}$, be arbitrary coefficients so that

$$\sum_{k=1}^{\infty} |c_k| \, \|L_k\| < \infty, \tag{5.2.7}$$

is satisfied. Then

$$\left(\sum_{k=1}^{\infty} c_k L_k u\right)_n = \left(2\sum_{k=1}^{\infty} c_k\right)u_n - \sum_{k=1}^{\infty} c_k(u_{n-k} + u_{n+k}).$$

Now the assertions of the lemma can be seen as follow;

For the Laplace transform we have

$$\begin{aligned} \left(\tilde{L}_{L,\lambda}u\right)_n &= \sum_{k=1}^{\infty} e^{-\lambda k}(2u_n - u_{n+k} - u_{n-k}) \\ &= 2\sum_{k=1}^{\infty} e^{-\lambda k}u_n - \sum_{k=1}^{\infty} e^{-\lambda k}(u_{n+k} + u_{n-k}) \\ &= \frac{2}{e^\lambda - 1}u_n - \sum_{k=1}^{\infty} e^{-\lambda k}(u_{n+k} + u_{n-k}). \end{aligned}$$

For the factorial transform we have

$$\begin{aligned}\left(\tilde{L}_{F,z}u\right)_n &= \sum_{k=1}^{\infty}\frac{z^k}{k!}(2u_n - u_{n+k} - u_{n-k}) \\ &= 2\sum_{k=1}^{\infty}\frac{z^k}{k!}u_n - \sum_{k=1}^{\infty}\frac{z^k}{k!}(u_{n+k} + u_{n-k}) \\ &= 2(e^z - 1)u_n - \sum_{k=1}^{\infty}\frac{z^k}{k!}(u_{n+k} + u_{n-k}).\end{aligned}$$

For the Mellin transform we have

$$\begin{aligned}\left(\tilde{L}_{M,s}u\right)_n &= \sum_{k=1}^{\infty}\frac{1}{k^s}(2u_n - u_{n+k} - u_{n-k}) \\ &= 2\sum_{k=1}^{\infty}\frac{1}{k^s}u_n - \sum_{k=1}^{\infty}\frac{1}{k^s}(u_{n+k} + u_{n-k}) \\ &= 2\zeta(s)u_n - \sum_{k=1}^{\infty}\frac{1}{k^s}(u_{n+k} + u_{n-k}),\end{aligned}$$

since

$$(L_k e_0)_n = 2\delta_{n,0} - \delta_{n,-k} - \delta_{n,k}.$$

Hence we have

$$\begin{aligned}\left(\tilde{L}_{L,\lambda}e_0\right)_n &= \tfrac{2}{e^\lambda - 1}\delta_{n,0} - \textstyle\sum_{k=1}^{\infty} e^{-\lambda k}(\delta_{n,-k} + \delta_{n,k}), \\ &= \begin{cases} \dfrac{2}{e^\lambda - 1} & \text{if } n = 0, \\ -e^{-\lambda|n|} & \text{if } n \neq 0, \end{cases}\end{aligned}$$

$$\begin{aligned}\left(\tilde{L}_{F,z}e_0\right)_n &= 2(e^z - 1)\delta_{n,0} - \textstyle\sum_{k=1}^{\infty}\frac{z^k}{k!}(\delta_{0,-k} + \delta_{0,k}), \\ &= \begin{cases} 2(e^z - 1) & \text{if } n = 0, \\ -\dfrac{z^{|n|}}{|n|!} & \text{if } n \neq 0, \end{cases}\end{aligned}$$

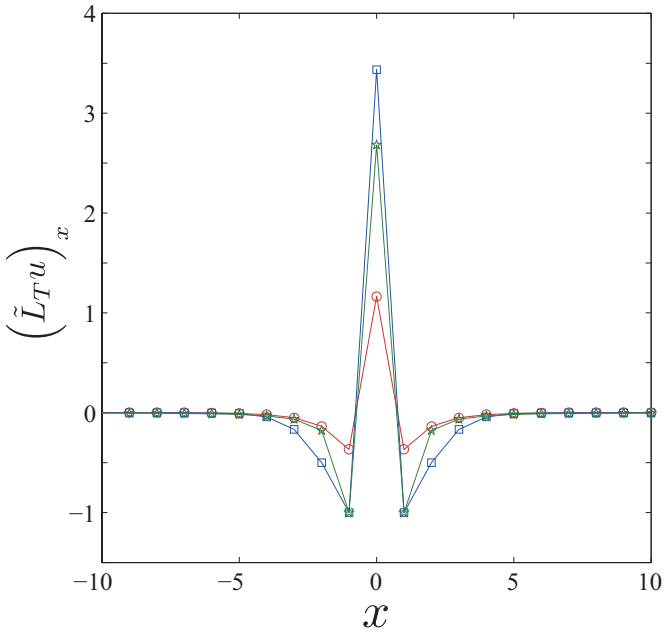


Figure 5.2.1: Plot of $(\tilde{L}_{L,\lambda}e_0)_x$, $(\tilde{L}_{F,z}e_0)_x$, and $(\tilde{L}_{M,s}e_0)_x$ at the different nodes of a linear path with 21 nodes obtained from the Laplace (circles), factorial (squares) and Mellin (stars) transformed k-path Laplacians with $\lambda = 1$, $z = 1$ and $s = 2.5$, respectively.

$$\begin{aligned}\left(\tilde{L}_{M,s}e_0\right)_n &= 2\zeta^{(s)}\delta_{n,0} - \textstyle\sum_{k=1}^{\infty} \frac{1}{k^s}(\delta_{0,-k} + \delta_{0,k}), \\ &= \begin{cases} 2\zeta(s) & \text{if } n = 0, \\ -\dfrac{1}{|n|^s} & \text{if } n \neq 0. \end{cases}\end{aligned}$$

□

Figure 5.2.1 illustrates the results of Lemma 5.1 in a graphical form displaying $\tilde{L}_{L,1}e_0$, $\tilde{L}_{F,1}e_0$ and $\tilde{L}_{M,2.5}e_0$ on 21 nodes. The plot clearly indicates that the three transforms of the k-path Laplacian operators hop the particles to distant sites in the linear chain.

5.3 Time-evolution operators

Time evolution is the change of state brought about by the passage of time, applicable to systems with internal state. In this formulation, time is not required

to be a continuous parameter, but may be discrete.

Let us now consider the time evolution of the particle density profile governed by the differential equation

$$\frac{d}{dt}u(t) = -Lu(t),$$

satisfying the initial equation $u(0) = w$, where L is any of the operators L_k, $\tilde{L}_{L,\lambda}$, $\tilde{L}_{F,z}$ or $\tilde{L}_{M,s}$, where $\lambda \in \mathbb{C}$ with $\Re\lambda > 0$, $z \in \mathbb{C}$, $s \in \mathbb{C}$ with $\Re s > 1$ and where $w \in \ell^2(P_\infty)$. Since L is a bounded operator in all cases, the solution is given by

$$u(t) = e^{-tL}w, \qquad t \geq 0. \tag{5.3.1}$$

To find this exponential operator e^{-tL}, we interpret sequences in $\ell^2(P_\infty)$ as Fourier coefficients and transform the problem into a problem in $L^2(-\pi, \pi)$. Define the unitary operator $\mathcal{F} : \ell^2(P_\infty) \to L^2(-\pi, \pi)$ by

$$(\mathcal{F}u)(q) = \frac{1}{\sqrt{2\pi}} \sum_{n\in\mathbb{Z}} u_n e^{inq}, \qquad u = (u_n)_{n\in\mathbb{Z}} \in \ell^2(P_\infty);$$

its inverse is given by

$$(\mathcal{F}^{-1}g)_n = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{-inq} g(q)dq, \qquad g \in L^2(-\pi, \pi).$$

Let us first determine the operator in $L^2(-\pi, \pi)$ that is equivalent to L_k via $\mathcal{F}$. For $u \in \ell^2(P_\infty)$ we have

$$\begin{aligned}
\big(\mathcal{F}L_k u\big)(q) &= \frac{1}{\sqrt{2\pi}} \sum_{n\in\mathbb{Z}} \big(2u_n - u_{n-k} - u_{n+k}\big)e^{inq} \\
&= \frac{1}{\sqrt{2\pi}} \sum_{n\in\mathbb{Z}} \big(2u_n e^{inq} - u_n e^{i(n+k)q} - u_n e^{i(n-k)q}\big) \\
&= \frac{1}{\sqrt{2\pi}} \sum_{n\in\mathbb{Z}} \big(2 - e^{ikq} - e^{-ikq}\big)u_n e^{inq} = \big(2 - e^{ikq} - e^{-ikq}\big)(\mathcal{F}u)(q).
\end{aligned}$$

Hence the operator L_k is unitarily equivalent to the multiplication operator in $L^2(-\pi,\pi)$ by the function

$$\ell_k(q) := 2 - e^{ikq} - e^{-ikq} = 2\big(1-\cos(kq)\big), \tag{5.3.2}$$

i.e.

$$\big(\mathcal{F}L_k\mathcal{F}^{-1}g\big)(q) = \ell_k(q)g(q), \qquad g \in L^2(-\pi,\pi). \tag{5.3.3}$$

The transformed operators $\tilde{L}_{L,\lambda}$, $\tilde{L}_{F,z}$ and $\tilde{L}_{M,s}$, are also unitarily equivalent to multiplication operators:

$$\big(\mathcal{F}\tilde{L}_k\mathcal{F}^{-1}g\big)(q) = \tilde{\ell}_T(q)g(q), \tag{5.3.4}$$

for $T = \mathrm{L}, \lambda$, $T = \mathrm{F}, z$ or $T = \mathrm{M}, s$ where

$$\begin{gathered}\tilde{\ell}_{L,\lambda}(q) := \sum_{k=1}^{\infty} e^{-\lambda k}\ell_k(q), \qquad \tilde{\ell}_{F,z}(q) := \sum_{k=1}^{\infty} \frac{z^k}{k!}\ell_k(q), \\ \tilde{\ell}_{M,s}(q) := \sum_{k=1}^{\infty} \frac{1}{k^s}\ell_k(q).\end{gathered} \tag{5.3.5}$$

Closed forms for these sums are given in the next lemma.

Lemma 5.2. *Let $\lambda \in \mathbb{C}$ with $\Re\lambda > 0$, $z \in \mathbb{C}$, $s \in \mathbb{C}$ with $\Re s > 1$. With the notation from above we have*

$$\tilde{\ell}_{L,\lambda}(q) = \frac{(e^{\lambda}+1)(1-\cos q)}{(e^{\lambda}-1)(\cosh\lambda - \cos q)}\,, \tag{5.3.6}$$

$$\tilde{\ell}_{F,z}(q) = 2\big[e^{z} - e^{z\cos q}\cos(z\sin q)\big], \tag{5.3.7}$$

$$\tilde{\ell}_{M,s}(q) = 2\zeta(s) - Li_s(e^{iq}) - Li_s(e^{-iq}), \tag{5.3.8}$$

where Li_s is the polylogarithm — also known as Jonquière's function — as defined in (1.8.1).

Moreover, the functions $\tilde{\ell}_{L,\lambda}$, $\tilde{\ell}_{F,z}$ *and* $\tilde{\ell}_{M,s}$ *are continuous on* $[-\pi,\pi]$ *and satisfy*

$$\ell(q) > 0 \qquad \textit{for } q \in [-\pi,\pi] \setminus \{0\}, \tag{5.3.9}$$

for $\ell = \tilde{\ell}_{L,\lambda}, \tilde{\ell}_{F,z}, \tilde{\ell}_{M,s}$ *when* $\lambda > 0$, $z > 0$, $s > 1$, *respectively.*

Proof. Representation (5.3.6) follows from

$$\tilde{\ell}_{L,\lambda}(q) = 2\sum_{k=1}^{\infty} e^{-\lambda k} - \sum_{k=1}^{\infty} e^{-\lambda k}e^{ikq} - \sum_{k=1}^{\infty} e^{-\lambda k}e^{-ikq}$$

$$\begin{aligned}
&= \frac{2}{e^{\lambda}-1} - \frac{1}{e^{\lambda-iq}-1} - \frac{1}{e^{\lambda+iq}-1} = \frac{2}{e^{\lambda}-1} - 2\frac{e^{\lambda}\cos q - 1}{\left|e^{\lambda-iq}-1\right|^2} \\
&= \frac{2}{e^{\lambda}-1} - 2\frac{e^{\lambda}\cos q - 1}{e^{2\lambda}+1-2e^{\lambda}\cos q} = \frac{2}{e^{\lambda}-1} - \frac{\cos q - e^{-\lambda}}{\cosh\lambda - \cos q} \\
&= \frac{(e^{\lambda}+1)(1-\cos q)}{(e^{\lambda}-1)(\cosh\lambda - \cos q)}\,.
\end{aligned}$$

The representation (5.3.7) follows from

$$\begin{aligned}
\tilde{\ell}_{F,z}(q) &= 2\sum_{k=1}^{\infty}\frac{z^k}{k!} - \sum_{k=1}^{\infty}\frac{z^k}{k!}e^{ikq} - \sum_{k=1}^{\infty}\frac{z^k}{k!}e^{-ikq} \\
&= 2(e^z-1) - \sum_{k=1}^{\infty}\frac{(ze^{iq})^k}{k!} - \sum_{k=1}^{\infty}\frac{(ze^{-iq})^k}{k!} \\
&= 2(e^z-1) - (e^{ze^{iq}}-1) - (e^{ze^{-iq}}-1) \\
&= 2[e^z - e^{z\cos q}\cos(z\sin g)].
\end{aligned}$$

The representation (5.3.8) follows from

$$\begin{aligned}\tilde{\ell}_{M,s}(q) &= 2\sum_{k=1}^{\infty}\frac{1}{k^s} - \sum_{k=1}^{\infty}\frac{1}{k^s}e^{ikq} - \sum_{k=1}^{\infty}\frac{1}{k^s}e^{-ikq} \\ &= 2\zeta(s) - \sum_{k=1}^{\infty}\frac{(e^{iq})^k}{k^s} - \sum_{k=1}^{\infty}\frac{(e^{-iq})^k}{k^s} \\ &= 2\zeta(s) - Li_s(e^{iq}) - Li_s(e^{-iq}).\end{aligned}$$

The continuity of the functions follows from the representations (5.3.6)–(5.3.8) or from the uniform convergence of the series. To show (5.3.9), observe that $\ell_k(q) = 2(1-\cos(kq)) \geq 0$ for all $q \in [-\pi,\pi]$. Moreover, $\ell_1(q) > 0$ for $q \in [-\pi,\pi] \setminus \{0\}$. Since all coefficients in the series in (5.3.5) are positive when $\lambda > 0$, $z > 0$, $s > 0$, respectively, the claim follows. □

The following theorem gives an explicit description of the time evolution operator corresponding to the transformed k-path Laplacians.

Theorem 5.3. *Let $\lambda \in \mathbb{C}$ with $\Re\lambda > 0$, $z \in \mathbb{C}$ and $s \in \mathbb{C}$ with $\Re s > 1$, let $L = L_k$, $\tilde{L}_{L,\lambda}$, $\tilde{L}_{F,z}$, or $\tilde{L}_{M,s}$ and let $\ell = \ell_k$,$\tilde{\ell}_{L,\lambda}$, $\tilde{\ell}_{F,z}$, $\tilde{\ell}_{M,s}$, correspondingly. For $w = (w_\nu)_{\nu\in\mathbb{Z}} \in \ell^2(P_\infty)$ the solution of (5.3.1) is given by*

$$\big(u(t)\big)_n = \big(e^{-tL}w\big)_n = \sum_{\nu\in\mathbb{Z}} w_\nu \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(n-\nu)q}e^{-t\ell(q)}dq, \qquad t \geq 0,\ n \in \mathbb{Z}. \tag{5.3.10}$$

The entries of the double-infinite Toeplitz matrix corresponding to the time evolution operator e^{-tL} are

$$\big(e^{-tL}\big)_{\mu\nu} = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(\mu-\nu)q}e^{-t\ell(q)}dq = \frac{1}{2\pi}\int_{-\pi}^{\pi}\cos\big((\mu-\nu)q\big)e^{-t\ell(q)}dq. \tag{5.3.11}$$

Proof. Since $\mathcal{F}L\mathcal{F}^{-1}$ acts as a multiplication operator by ℓ (see (5.3.3) and

(5.3.4)), we have

$$\begin{aligned}\left(\mathcal{F}e^{-tL}\mathcal{F}^{-1}g\right)(q) &= \sum_{n=0}^{\infty}(\mathcal{F}\,\frac{(-1)^n t^n L^n}{n!}\,\mathcal{F}^{-1}g)(q)\\ &= \sum_{n=0}^{\infty}\frac{1}{\sqrt{2\pi}}\sum_{k\in\mathbb{Z}}e^{-iq}(\frac{(-1)^n t^n L^n}{n!}\,\mathcal{F}^{-1}g(q))_k\\ &= \sum_{n=0}^{\infty}\frac{(-1)^n t^n}{n!}\,(\mathcal{F}L^n\mathcal{F}^{-1}g)(q)) = \sum_{n=0}^{\infty}\frac{(-1)^n t^n}{n!}\,\ell(q)^n g(q)\\ &= e^{-t\ell(q)}g(q), \qquad g\in L^2(-\pi,\pi).\end{aligned}$$

Let $\nu\in\mathbb{Z}$ and e_ν as in (4.2.8). Then

$$\begin{aligned}\left(e^{-tL}e_\nu\right)_n &= \left(\mathcal{F}^{-1}e^{-t\ell(\cdot)}\mathcal{F}e_\nu\right)_n = \frac{1}{\sqrt{2\pi}}\int_{-\pi}^{\pi}e^{-inq}e^{-t\ell(q)}\frac{1}{\sqrt{2\pi}}e^{i\nu q}dq\\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi}e^{-i(n-\nu)q}e^{-t\ell(q)}dq = \frac{1}{2\pi}\int_{-\pi}^{\pi}e^{i(n-\nu)q}e^{-t\ell(q)}dq,\end{aligned}$$

where the last equality follows since ℓ is an even function. Since e^{-tL} is a bounded operator we have

$$e^{-tL}w = \sum_{\nu\in\mathbb{Z}}w_\nu e^{-tL}e_\nu,$$

which proves (5.3.10) and hence also (5.3.11). □

In Figure 5.3.1 we illustrate the time evolution of the density $u(t)$ for the three transforms of the k-path Laplace operators.

Remark 5.4. For a similar representation for the case $L = L_1$, the discrete Laplacian L acts as follows

$$(Lu)_n = 2u_n - u_{n+1} - u_{n-1},\ n\in\mathbb{Z}, \tag{5.3.12}$$

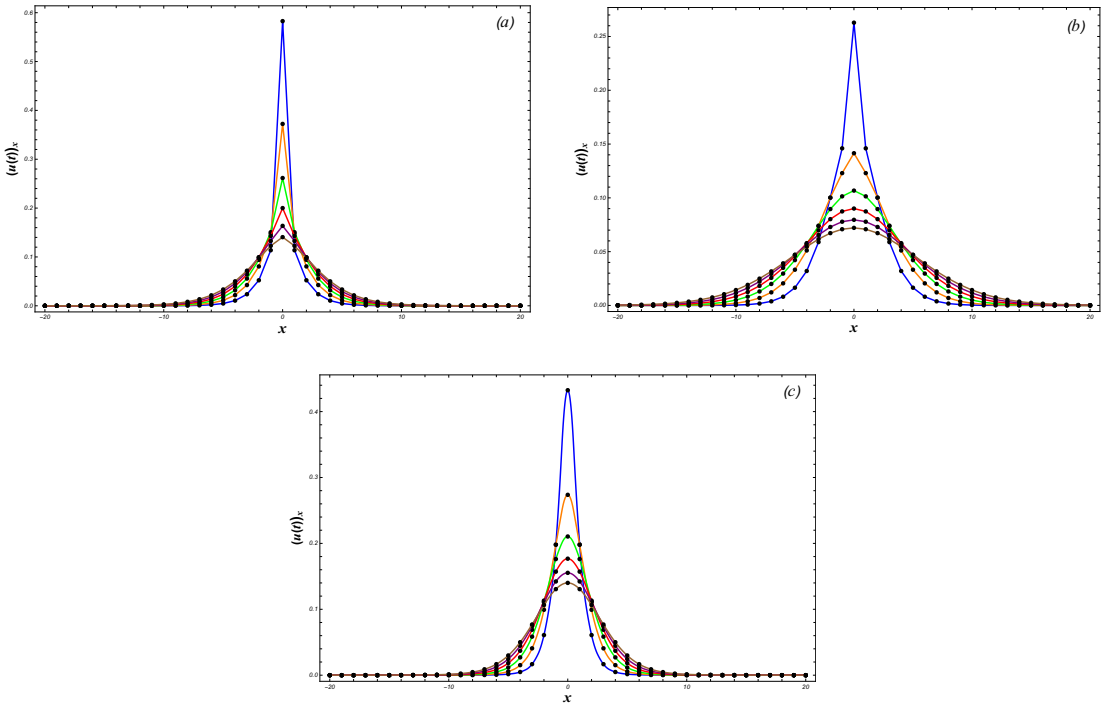


Figure 5.3.1: The particle density $(u(t))_x$ as a function of x for the transformed k-path Laplacians for a linear chain with 41 nodes. The symbols indicate the results obtained from the simulations of the linear chain and the solid lines connect the points for better visibility for different time: $t = 0.5$ (circles), $t = 1.0$ (squares), $t = 1.5$ (dots), $t = 2.0$ (rhombus), $t = 2.5$ (triangles), $t = 3.0$ (stars). (a) Laplace transform with $\lambda = 1$. (b) Factorial-transform with $z = 1$. (c) Mellin-transform with $s = 4$.

and the fundamental solution of equation above is given by

$$(u(t))_n = \exp(-2t)\, I_{n-m}(2t),\ t \geq 0,$$

where I_k is the modified Bessel function of the first kind and other $k \in \mathbb{Z}$, defined as

$$I_k(t) = \sum_{m=0}^{\infty} \frac{1}{\Gamma(m+k+1)} (\frac{t}{2})^{2m+k}.$$

Consequently, the unique solution of the discrete Laplacian is described by the formal series

$$\exp(tL)u_n = \sum_{m \in \mathbb{Z}} \exp(2t)\, I_{n-m}(2t) u_m. \tag{5.3.13}$$

It was proved that $\{\exp(tL)\}_{t \geq 0}$ is a positive Markovian diffusion semigroup [**?**].

Here and in the following we use the following notation: let g_1 and g_2 be functions that are defined and positive-valued on an interval of the form (a, ∞); we write

$$g_1(x) \sim g_2(x) \qquad \text{as } x \to \infty \qquad\qquad \text{if} \qquad \lim_{x \to \infty} \frac{g_1(x)}{g_2(x)} = 1;$$

a similar notation is used for the behaviour as $x \to 0$.

5.4 Generalized diffusion on the path graph

In this section we prove that the density profile $u(t)$ that solves

$$\frac{d}{dt} u(t) = -Lu(t), \tag{5.4.1}$$

$$u(0) = e_0, \tag{5.4.2}$$

where e_0 is as in (5.2.4) and L is any of the transformed k-path Laplacians $\tilde{L}_{L,\lambda}$, $\tilde{L}_{F,z}$, or $\tilde{L}_{M,s}$, approaches a stable distribution if appropriately scaled.

In the following we study the asymptotic behaviour of the density profile $u(t)$

that solves (5.4.1) and (5.4.2). It follows from (5.3.10) that

$$\big(u(t)\big)_x = \big(e^{-tL}e_0\big)_x = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ixq}e^{-t\ell(q)}dq \qquad x\in\mathbb{Z},\, t\geq 0. \tag{5.4.3}$$

In the next lemma we consider the asymptotic behaviour of integrals as in (5.4.3). Relation (2.6.1) implies that $S(\alpha,0,\gamma,0)$ has no finite variance if $\alpha<2$. Further, if $\alpha\leq 1$, then even the first moment is infinite. We allow also values $\alpha>2$ in the notation $f(z;\alpha,0,\gamma,0)$ although this is not needed later.

Lemma 5.5. *Let $\alpha>0$ and let $h:[-\pi,\pi]\to\mathbb{R}$ be a continuous function that satisfies*

$$h(q)>0 \qquad \text{for } q\in[-\pi,\pi]\setminus\{0\}, \tag{5.4.4}$$

$$h(q)\sim c|q|^\alpha \qquad \text{as } q\to 0, \tag{5.4.5}$$

with some $c>0$. Then

$$t^{\frac{1}{\alpha}}\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{it^{\frac{1}{\alpha}}\xi q}e^{-th(q)}dq \to \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\xi z}e^{-c|z|^\alpha}dz \tag{5.4.6}$$

$$= f\big(\xi;\alpha,0,c^{\frac{1}{\alpha}},0\big), \tag{5.4.7}$$

uniformly in ξ on $\mathbb{R}$ as $t\to\infty$.

Hence

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ixq}e^{-th(q)}dq = t^{-\frac{1}{\alpha}}f\big(t^{-\frac{1}{\alpha}}x;\alpha,0,c^{\frac{1}{\alpha}},0\big)+o\big(t^{-\frac{1}{\alpha}}\big), \tag{5.4.8}$$

uniformly in $x\in\mathbb{R}$ as $t\to\infty$.

Proof. Let $t > 0$. With the substitution $z = t^{\frac{1}{\alpha}} q$ we have

$$\left| t^{\frac{1}{\alpha}} \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{it^{\frac{1}{\alpha}}\xi q} e^{-th(q)} dq - \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi z} e^{-c|z|^\alpha} dz \right|$$

$$= \left| \frac{1}{2\pi} \int_{-\pi t^{\frac{1}{\alpha}}}^{\pi t^{\frac{1}{\alpha}}} e^{i\xi z} e^{-th(t^{-\frac{1}{\alpha}} z)} dz - \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi z} e^{-c|z|^\alpha} dz \right|$$

$$\leq \left| \frac{1}{2\pi} \int_{-\pi t^{\frac{1}{\alpha}}}^{\pi t^{\frac{1}{\alpha}}} e^{i\xi z} \left(e^{-th(t^{-\frac{1}{\alpha}} z)} - e^{-c|z|^\alpha} \right) dz \right|$$

$$+ \left| \frac{1}{2\pi} \int_{\mathbb{R}\setminus[-\pi t^{\frac{1}{\alpha}}, \pi t^{\frac{1}{\alpha}}]} e^{i\xi z} e^{-c|z|^\alpha} dz \right|$$

$$\leq \frac{1}{2\pi} \int_{-\pi t^{\frac{1}{\alpha}}}^{\pi t^{\frac{1}{\alpha}}} \left| e^{-th(t^{-\frac{1}{\alpha}} z)} - e^{-c|z|^\alpha} \right| dz \tag{5.4.9}$$

$$+ \frac{1}{2\pi} \int_{\mathbb{R}\setminus[-\pi t^{\frac{1}{\alpha}}, \pi t^{\frac{1}{\alpha}}]} e^{-c|z|^\alpha} dz. \tag{5.4.10}$$

First note that the integrals in (5.4.9) and (5.4.10) are independent of ξ. We show that both integrals converge to 0 as $t \to \infty$. For the integral in (5.4.10) this is clear. Let us now consider the integral in (5.4.9). Since h is continuous and satisfies (5.4.4) and (5.4.5), the function $q \mapsto h(q)/|q|^\alpha$ is bounded below by a positive constant, i.e. there exists $\tilde{c} > 0$ such that

$$\frac{h(q)}{|\ q\ |^\alpha} > \tilde{c} \text{ for } q \in [\pi,\ \pi];$$

i.e.

$$h(q) \geq \tilde{c}|q|^\alpha \qquad \text{for } \ q \in [-\pi, \pi].$$

This implies that the integrand in (5.4.9) satisfies

$$\begin{aligned}\left|e^{-th(t^{-\frac{1}{\alpha}}z)}-e^{-c|z|^\alpha}\right| &\le e^{-th(-t^{-\frac{1}{\alpha}}z)}+e^{-c|z|^\alpha}\\ &\le e^{-t\tilde{c}|t^{-\frac{1}{\alpha}}z|^\alpha}+e^{-c|z|^\alpha}=e^{-\tilde{c}|z|^\alpha}+e^{-c|z|^\alpha},\end{aligned}$$

for $z \in [-\pi t^{\frac{1}{\alpha}}, \pi t^{\frac{1}{\alpha}}]$. Therefore the integrand in (5.4.9) is bounded by the integrable function $z \mapsto e^{-\tilde{c}|z|^\alpha} + e^{-c|z|^\alpha}$, which is independent of t. For fixed $z \in \mathbb{R}$ we have

$$th\big(t^{-\frac{1}{\alpha}}z\big) = |z|^\alpha \frac{h(t^{-\frac{1}{\alpha}}z)}{|t^{-\frac{1}{\alpha}}z|^\alpha} \to c|z|^\alpha \qquad \text{as } t \to \infty,$$

by (5.4.5) and hence

$$\left|e^{-th(t^{-\frac{1}{\alpha}}z)}-e^{-c|z|^\alpha}\right| \to 0 \qquad \text{as } t \to \infty.$$

Now the Dominated Convergence Theorem implies that the integral in (5.4.9) converges to 0 as $t \to \infty$. This shows (5.4.6).

Finally, we prove (5.4.8). With the substitution $x = t^{\frac{1}{\alpha}}\xi$ we obtain from (5.4.6) and (5.4.7) that

$$\begin{aligned}&\frac{1}{t^{-\frac{1}{\alpha}}}\left|\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ixq}e^{-th(q)}\,dq - t^{-\frac{1}{\alpha}} f\big(t^{-\frac{1}{\alpha}}x;\alpha,0,c^{\frac{1}{\alpha}},0\big)\right|\\ &= \left|t^{\frac{1}{\alpha}}\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ixq}e^{-th(q)}\,dq - f\big(t^{-\frac{1}{\alpha}}x;\alpha,0,c^{\frac{1}{\alpha}},0\big)\right| \to 0,\end{aligned}$$

uniformly in $x \in \mathbb{R}$ as $t \to \infty$, which shows (5.4.8). □

Remark 5.6. The lemma can be interpreted as follows. If the function

$$g(x,t) := \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ixq}e^{-th(q)}dq,$$

is scaled in the independent and the dependent variable, then it converges:

$$t^{\frac{1}{\alpha}} g\big(t^{\frac{1}{\alpha}}\xi, t\big) \to f\big(\xi; \alpha, 0, c^{\frac{1}{\alpha}}, 0\big) \qquad \text{as } \; t \to \infty.$$

This means that the profile spreads proportionally to $t^{\frac{1}{\alpha}}$. The solution $(u(t))_x$ is defined only for $x \in \mathbb{Z}$. Scaling this discrete profile in the same way leads to a sequence of points:

$$\Big(t^{-\frac{1}{\alpha}} x, t^{\frac{1}{\alpha}} \big(u(t)\big)_x\Big) \qquad x \in \mathbb{Z},$$

for each $t \geq 0$; the points lie on the graph of the function $\xi \mapsto t^{\frac{1}{\alpha}} g(t^{\frac{1}{\alpha}}\xi, t)$. These sequences of points become denser as t growths and converge to the limiting profile $f(\xi; \alpha, 0, c^{\frac{1}{\alpha}}, 0)$ as $t \to \infty$. In particular, the maximum height, which is attained at 0, decreases like

$$\big(u(t)\big)_0 \sim t^{-\frac{1}{\alpha}} f\big(0; \alpha, 0, c^{\frac{1}{\alpha}}, 0\big) = \frac{\Gamma\big(\frac{\alpha+1}{\alpha}\big)}{\pi c^{\frac{1}{\alpha}}} t^{-\frac{1}{\alpha}} \qquad \text{as } \; t \to \infty. \tag{5.4.11}$$

The full width at half maximum (FWHM) increases like

$$FWHM(t) \sim 2\xi_0 t^{\frac{1}{\alpha}} \qquad \text{as } \; t \to \infty, \tag{5.4.12}$$

where $\xi_0 > 0$ is such that $f(\xi_0; \alpha, 0, c^{\frac{1}{\alpha}}, 0) = \frac{1}{2} f(0; \alpha, 0, c^{\frac{1}{\alpha}}, 0)$. This implies that if $\alpha = 2$, then one has normal diffusion, and if $\alpha < 2$, then the time evolution is superdiffusive since $(FWHM(t))^2 \sim ct^{\kappa}$ with $\kappa = \frac{2}{\alpha}$. We used the square of the full width at half maximum $FWHM^2$ instead of the mean square displacement MSD because the latter is infinite if $\alpha < 2$.

5.4.1 Diffusion for the Laplace- and factorial-transformed k-path Laplacians

In the next theorem we show that the time evolution with the k-path Laplacians and the Laplace-transformed and factorial-transformed k-path Laplacians show normal diffusion (see, e.g. [31] for the case $L = L_1$). This is caused by the fact that ℓ_k, $\tilde{\ell}_{L,\lambda}$ and $\tilde{\ell}_{F,z}$ behave quadratically around 0 (see Fig 5.4.1).

Theorem 5.7. *Let P_∞ be the infinite path graph, let $\lambda, z > 0$ and let $\tilde{L}_{L,\lambda}$ and $\tilde{L}_{F,z}$ be the Laplace-transformed and factorial-transformed k-path Laplacian with parameters λ and z, respectively. Moreover, let $u(t)$ be the solution of* (5.4.1), (5.4.2) *with $L = L_k$, $L = \tilde{L}_{L,\lambda}$ or $L = \tilde{L}_{F,z}$. Then*

$$\big(u(t)\big)_x = t^{-\frac{1}{2}} \frac{1}{2\sqrt{\pi a}} \exp\left(-\frac{x^2}{4at}\right) + o\big(t^{-\frac{1}{2}}\big) \qquad as\ \ t \to \infty, \tag{5.4.13}$$

uniformly in $x \in \mathbb{Z}$ where

$$a = k^2 \qquad for\ \ L = L_k, \tag{5.4.14}$$

$$a = \frac{e^\lambda \left(e^\lambda + 1\right)}{(e^\lambda - 1)^3} = \frac{\coth\big(\frac{\lambda}{2}\big)}{2(\cosh\lambda - 1)} \qquad for\ \ L = \tilde{L}_{L,\lambda}, \tag{5.4.15}$$

$$a = z(z+1)e^z \qquad for\ \ L = \tilde{L}_{F,z}. \tag{5.4.16}$$

Proof. From (5.3.2),

$$\lim_{q\to 0} \frac{2(1-\cos(kq)}{aq^2} \le \lim_{q\to 0} \frac{k\sin(kq)}{aq}$$
$$= \lim_{q\to 0} \frac{k^2\cos(kq)}{a}.$$

Hence, with $a = k^2$, the asymptotic behaviour of the functions ℓ_k is $\ell_k(q) \sim k^2q^2 as\, q \to 0$,

Also, from(5.3.6),

$$\begin{aligned}\lim_{q\to 0}\frac{(e^\lambda+1)(1-\cos q)}{(e^\lambda-1)(\cosh\lambda-\cos q)\,aq^2} &= \frac{e^\lambda+1}{e^\lambda-1}\lim_{q\to 0}\frac{(1-\cos q)}{(\cosh\lambda-\cos q)}\,aq^2\\ &= \frac{e^\lambda+1}{e^\lambda-1}\lim_{q\to 0}\frac{\sin q}{2a\,\cosh\lambda q+a\sin q^2-2aq\,\cos q}\\ &= \frac{e^\lambda+1}{e^\lambda-1}\frac{1}{2a(\cosh\lambda-1)}.\end{aligned}$$

With, $a=\frac{(e^\lambda+1)e^\lambda}{(e^\lambda-1)^3}$, the asymptotic behaviour of the functions $\tilde{\ell}_{L,\lambda}$is

$$\tilde{\ell}_{L,\lambda}(q)=\frac{e^\lambda+1}{(e^\lambda-1)(\cosh\lambda-1)}\cdot\frac{q^2}{2}+O\big(q^4\big)=aq^2+O\big(q^4\big)\qquad\text{as }\ q\to 0.$$

And from (5.3.7)

$$\lim_{q\to 0}\frac{2[e^z-e^{z\cos q}\cos(z\sin q)]}{aq^2}=z(1-z)e^z.$$

With, $a=z(1-z)e^z$, we obtain that the asymptotic behaviour of the functions $\tilde{\ell}_{F,z}$ is

$$\begin{aligned}\tilde{\ell}_{F,z}(q) &= 2\left[e^z-e^z\left(1-\frac{zq^2}{2}+O\big(q^4\big)\right)\left(1-\frac{z^2q^2}{2}+O\big(q^4\big)\right)\right]\\ &= e^z(z+z^2)q^2+O\big(q^4\big)\qquad\text{as }\ q\to 0,\end{aligned}$$

with a from (5.4.16), respectively (see Fig. 5.4.2) . Now (5.4.13) follows from (5.4.3) and Lemma 5.5. □

Remark 5.8. Theorem 5.7 shows that the diffusion for the k-path Laplacian, the Laplace-transformed and the factorial-transformed k-path Laplacian is always

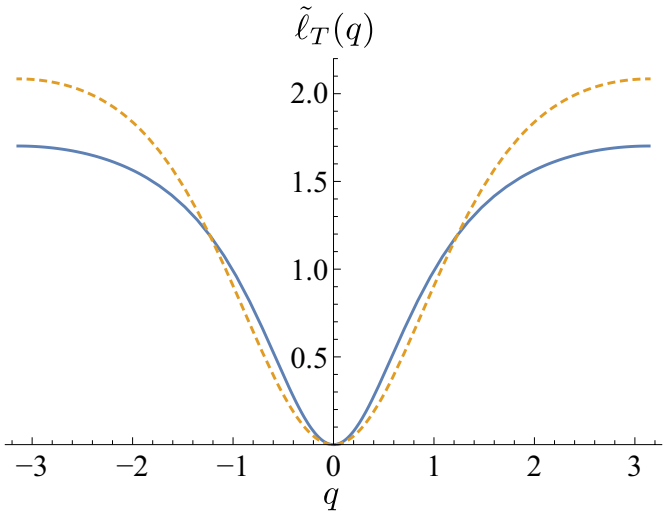


Figure 5.4.1: The graphs of the functions $\tilde{\ell}_{L,\lambda}$ with $\lambda = 1$ (blue solid curve) and $\tilde{\ell}_{F,z}$ with $z = 1/2$ (orange broken curve) on the interval $[-\pi, \pi]$.

normal. The peak height of the distribution is attained at $x = 0$ and behaves like

$$\big(u(t)\big)_0 \sim \frac{1}{2\sqrt{\pi a}} t^{-\frac{1}{2}} \qquad \text{as } \ t \to \infty,$$

where a is from (5.4.14)–(5.4.16); see (5.4.11). The mean square displacement behaves like

$$\mathrm{MSD}(t) \sim 2at \qquad \text{as } \ t \to \infty,$$

and the full width at half maximum (FWHM) behaves like

$$FWHM(t) \sim 2\sqrt{(\ln 2)a}\, t^{\frac{1}{2}} \qquad \text{as } \ t \to \infty;$$

see (5.4.12). For the limiting behaviour after rescaling in x see Remark 5.6.

5.4.2 Diffusion for the Mellin-transformed k-path Laplacian

For the Mellin-transformed k-path Laplacian, the density profile shows superdiffusion for $1 < s < 3$ and normal diffusion for $s > 3$; see Fig 5.4.3.

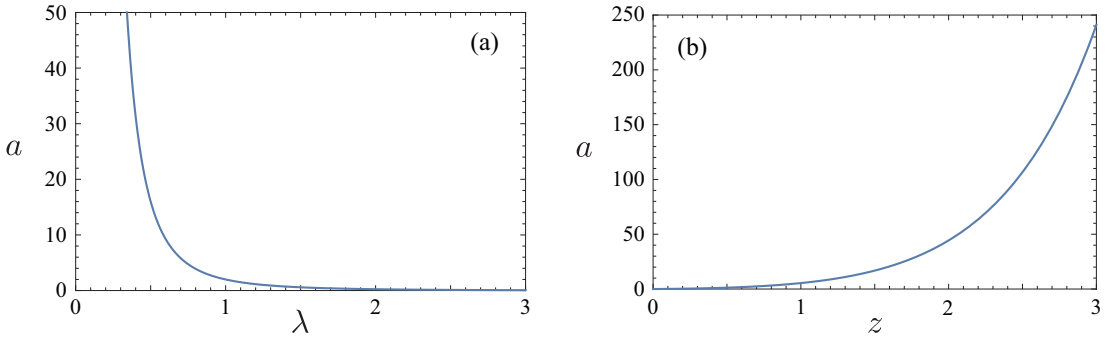


Figure 5.4.2: The parameter dependence of a for (a) the Laplace-transformed and (b) the factorial-transformed k-path Laplacian.

Theorem 5.9. *Let P_∞ be the infinite path graph, let $s > 1$ and let $\tilde{L}_{M,s}$ be the Mellin-transformed k-path Laplacian with parameter s. Moreover, let $u(t)$ be the solution of (5.4.1) and (5.4.2) with $L = \tilde{L}_{M,s}$. Then*

$$\big(u(t)\big)_x = t^{-\frac{1}{\alpha}} f\big(t^{-\frac{1}{\alpha}} x; \alpha, 0, \gamma, 0\big) + o\big(t^{-\frac{1}{\alpha}}\big) \qquad \text{as } t \to \infty, \tag{5.4.17}$$

uniformly in $x \in \mathbb{Z}$ where

$$\alpha = s - 1, \quad \gamma = \left(-\frac{\pi}{\Gamma(s) \cos\big(\frac{\pi s}{2}\big)} \right)^{\frac{1}{s-1}} \qquad \text{if } 1 < s < 3, \tag{5.4.18}$$

$$\alpha = 2, \qquad \gamma = \sqrt{\zeta(s-2)} \qquad \text{if } s > 3. \tag{5.4.19}$$

In the case $1 < s < 3$, the (rescaled) limit distribution has the following asymptotic behaviour:

$$f(\xi; \alpha, 0, \gamma, 0) \sim \frac{1}{\xi^s} \qquad \text{as } \xi \to \pm\infty, \tag{5.4.20}$$

where α and γ are defined in (5.4.18).

Note that in the case when $s > 3$ the limiting distribution is a normal distribution and hence

$$\big(u(t)\big)_x = t^{-\frac{1}{2}} \frac{1}{2\sqrt{\pi\zeta(s-2)}} \exp\left(-\frac{x^2}{4\zeta(s-2)t} \right) + o\big(t^{-\frac{1}{2}}\big) \qquad \text{as } t \to \infty;$$

when $s = 2$, the limiting distribution is a Cauchy distribution and hence

$$\big(u(t)\big)_x = \frac{t}{x^2 + \pi^2 t^2} + o\big(t^{-1}\big) \qquad \text{as } t \to \infty.$$

Proof. We consider the behaviour of $\tilde{\ell}_{M,s}$ from (5.3.8) at 0. Let $s > 1$ with $s \notin \mathbb{N}$. It follows from (1.8.3) that

$$Li_s(e^z) = \Gamma(1-s)(-z)^{s-1} + \sum_{n=0}^{\infty} \zeta(s-n)\frac{z^n}{n!}, \qquad |z| < 2\pi,\ z \notin (0,\infty),$$

which yields

$$\begin{aligned}
\tilde{\ell}_{M,s}(q) &= 2\zeta(s) - Li_s(e^{iq}) - Li_s(e^{-iq}) \\
&= 2\zeta(s) - \Gamma(1-s)\Big((-iq)^{s-1} + (iq)^{s-1}\Big) - \sum_{n=0}^{\infty} \zeta(s-n)\frac{(iq)^n + (-iq)^n}{n!} \\
&= -\Gamma(1-s)|q|^{s-1}\Big(e^{-i(s-1)\frac{\pi}{2}} + e^{i(s-1)\frac{\pi}{2}}\Big) - \sum_{n=1}^{\infty} \zeta(s-n)\frac{(iq)^n + (-iq)^n}{n!} \\
&= -\frac{\pi}{\Gamma(s)\sin(\pi s)}|q|^{s-1} 2\cos\left(\frac{(s-1)\pi}{2}\right) - \sum_{l=1}^{\infty} \zeta(s-2l)\frac{2(-1)^l q^{2l}}{(2l)!} \\
&= -\frac{\pi}{\Gamma(s)\cos\big(\frac{s\pi}{2}\big)}|q|^{s-1} - \sum_{l=1}^{\infty} \zeta(s-2l)\frac{2(-1)^l q^{2l}}{(2l)!} \qquad (5.4.21) \\
&= -\frac{\pi}{\Gamma(s)\cos\big(\frac{s\pi}{2}\big)}|q|^{s-1} + \zeta(s-2)q^2 + o(q^4), \qquad \text{as } q \to 0. \qquad (5.4.22)
\end{aligned}$$

By continuity (5.4.21) and hence (5.4.22) are also valid for $s = 2$. If $s < 3$, then the first term in (5.4.22) is dominating; if $s > 3$, then the second term is dominating. Hence

$$\tilde{\ell}_{M,s}(q) \sim \begin{cases} -\dfrac{\pi}{\Gamma(s)\cos\big(\frac{s\pi}{2}\big)}|q|^{s-1} & \text{if } 1 < s < 3, \\ \\ \zeta(s-2)q^2 & \text{if } s > 3, \end{cases}$$

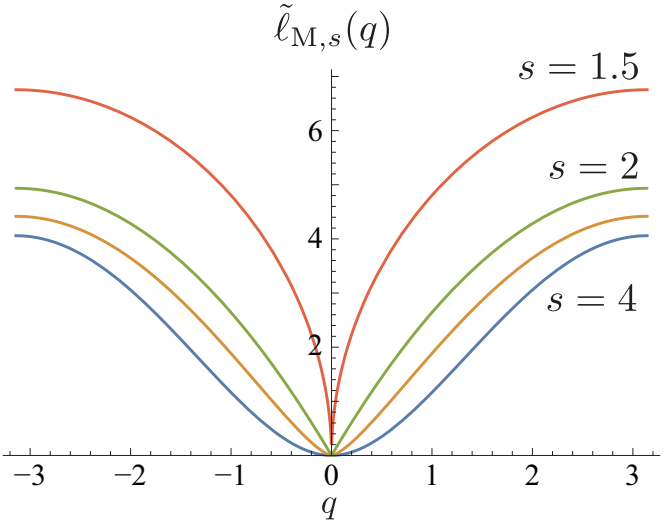


Figure 5.4.3: The graphs of the functions $\tilde{\ell}_{M,s}$ on the interval $[-\pi, \pi]$. The parameter s is varied from top to the bottom as 1.5, 2, 2.5 (not labelled) and 4.

as $q \to 0$. Now (5.4.17) follows from (5.4.3) and Lemma 5.5.

To show (5.4.20), we use (2.6.1), which yields

$$f(\xi; s-1, 0, \gamma, 0) \sim \frac{1}{\pi}\Gamma(s)\sin\left(\frac{\pi(s-1)}{2}\right)\frac{-\pi}{\Gamma(s)\cos\left(\frac{\pi s}{2}\right)} \cdot \frac{1}{\xi^s} = \frac{1}{\xi^s},$$

as $\xi \to \pm\infty$. □

When $s = 3$, the asymptotic expansion of $\tilde{\ell}_{M,s}(q)$ involves a logarithmic term, which implies that the asymptotic behaviour of $(u(t))_x$ is more complicated (see Fig 5.4.3).

Remark 5.10. In Fig. 5.4.4 we plot the density profiles for various times when the time evolution is governed by (5.4.1) with L being the Mellin-transformed k-path Laplacian $\tilde{L}_{M,s}$. The peak height is attained at $x = 0$ and behaves like

$$\big(u(t)\big)_0 \sim \begin{cases} \dfrac{\Gamma\left(\frac{s}{s-1}\right)}{\pi\gamma}\, t^{-\frac{1}{s-1}} & \text{if } \ 1 < s < 3, \\[2ex] \dfrac{1}{2\sqrt{\pi\zeta(s-2)}}\, t^{-\frac{1}{2}} & \text{if } \ s > 3, \end{cases}$$

as $t \to \infty$, where γ is as in (5.4.18); see (5.4.11). If $s \in (1, 3)$, then the full width

at half maximum (FWHM) behaves like

$$FWHM(t) \sim 2\xi_0 t^{\frac{1}{s-1}} \qquad \text{as } t \to \infty,$$

where $\xi_0 > 0$ is such that $f(\xi_0; s-1, 0, \gamma, 0) = \frac{1}{2} f(0; s-1, 0, \gamma, 0)$; see (5.4.12). This shows that we have superdiffusion in this case since $\frac{1}{s-1} > \frac{1}{2}$. A particular case is when $s = 2$, when the (rescaled) limit distribution is a Cauchy distribution and the FWHM grows linearly, i.e. the time evolution shows ballistic diffusion. For an interpretation of the limiting behaviour using rescaling in x see Remark 5.6 (see Fig.5.4.5).

Remark 5.11. Consider the operator

$$L = cL_1^a, \tag{5.4.23}$$

with $c > 0$ and $a \in (0, 1)$, i.e. L_1^a is a fractional power of the standard Laplacian L_1 defined, e.g. by the spectral theorem. Since the operator cL_1^a is equivalent to the multiplication operator by

$$\ell(q) = c\big(2(1 - \cos q)\big)^a,$$

in the Fourier representation, we obtain from Lemma 5.5 that

$$\big(u(t)\big)_x = t^{-\frac{1}{2a}} f\big(t^{-\frac{1}{2a}} x; 2a, 0, c^{\frac{1}{2a}}, 0\big) + o\big(t^{-\frac{1}{2a}}\big) \qquad \text{as } t \to \infty,$$

when u is a solution of (5.4.1), (5.4.2) with L as in (5.4.23). Hence if we choose

$$a = \frac{s-1}{2} \qquad \text{and} \qquad c = -\frac{\pi}{\Gamma(s)\cos\big(\frac{\pi s}{2}\big)},$$

for $s \in (1, 3)$, we obtain the same asymptotic behaviour of u as the solution in Theorem 5.9. However, the solutions behave differently for small t as can be seen

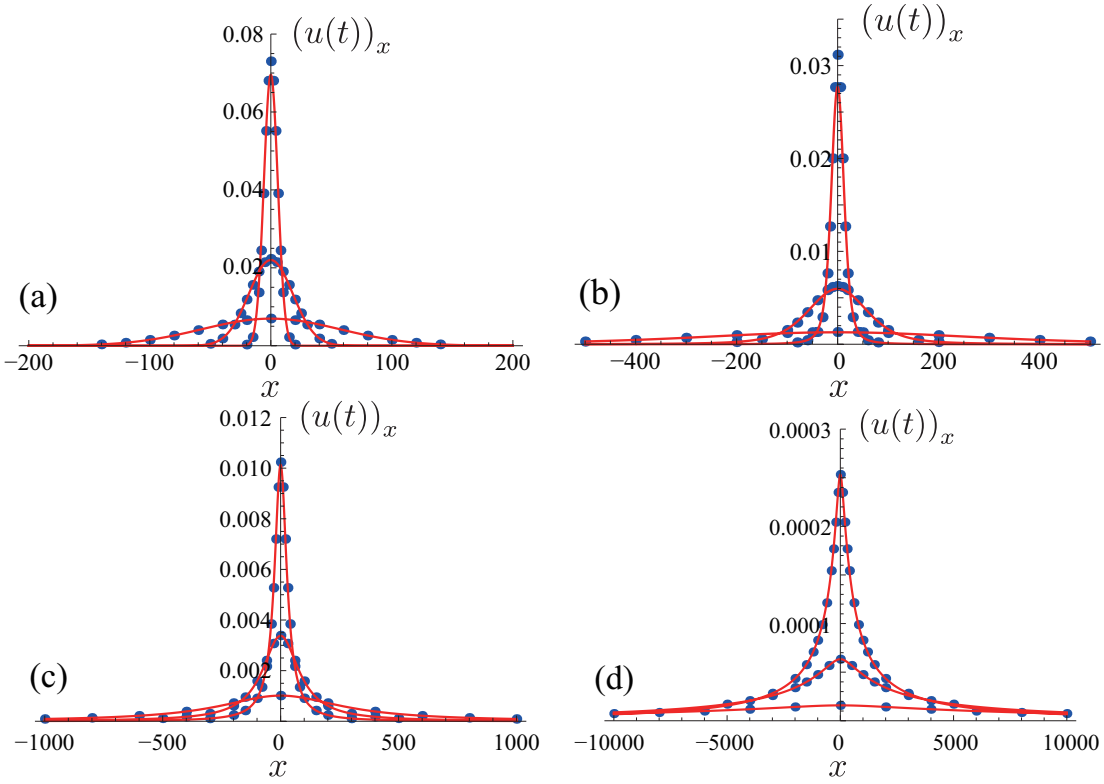


Figure 5.4.4: The time evolution of the density profile under the Mellin-transformed k-path Laplacian: (a) $s = 4$ for $t = 10, 100, 1000$ from high to low; (b) $s = 2.5$ for $t = 10, 100, 1000$ from high to low; (c) $s = 2$ for $t = 10, 30, 100$ from high to low; (d) $s = 1.5$ for $t = 10, 20, 40$ from high to low. In every panel, the blue dots indicate the result of numerical integration of (5.4.3) with $\ell = \tilde{\ell}_{M,s}$, whereas the red curves indicate the asymptote (5.4.17).

from Figure 5.4.6 where the blue solid line with circles corresponds to $L = \tilde{L}_{M,s}$ and the red dashed line with squares corresponds to $L = cL_1^a$ for $t = 1$ (a) and $t = 3$ (b). See [24] for a discussion of L_1^a where it was also shown that (5.4.1), (5.4.2) with $L = L_1^a$ is equivalent to an evolution equation with a fractional time derivative ([24, Theorem 3]).

5.5 Summary

As mentioned in the introduction, the aim of this study was the generalisation of the diffusion equation, controlled by the k-path LOs. This chapter has focussed upon a generalised diffusion equation where the transformed generalised k-path

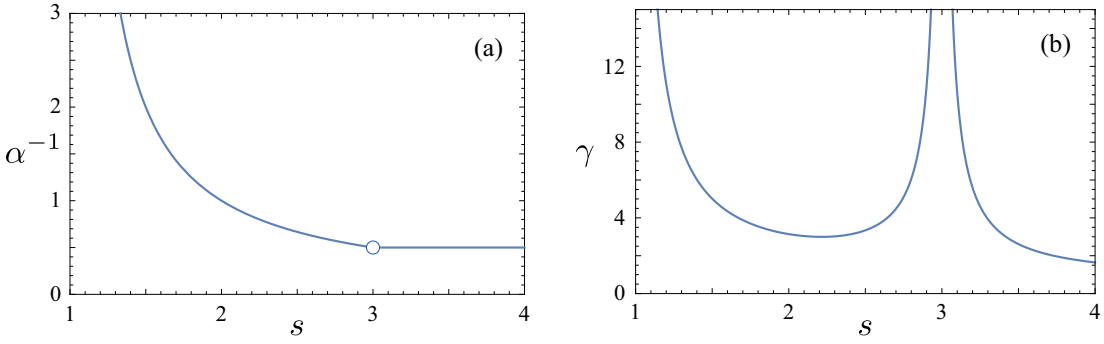


Figure 5.4.5: The s-dependence of (a) $1/\alpha$ and (b) γ.

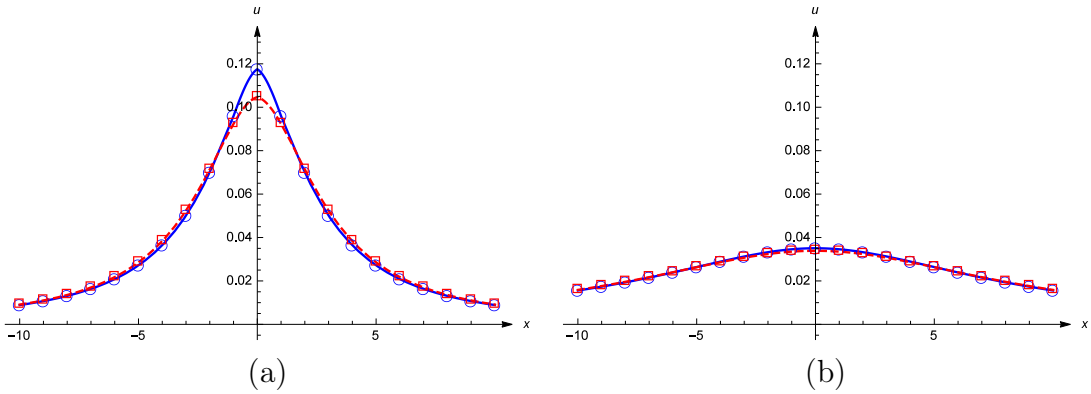


Figure 5.4.6: The solutions of (5.4.1), (5.4.2) for $L = \tilde{L}_{M,s}$ (blue solid line with circles) and for $L = cL_1^a$ (red dashed line with squares) for $t = 1$ (a) and $t = 3$ (b).

LOs for locally finite infinite networks are used. These generalised Laplacian operators are inserted into the graph-theoretic diffusion equation (5.2.1–5.2.2) to obtain a generalised diffusion equation for graphs. We have presented new methods to describe superdiffusion by a transformation of k-path LOs defined on the infinite path graph. Our analysis here proves that under the Mellin transform of these k-path LOs for certain values of the parameter, $1 < s < 3$, a superdiffusive dynamic appears (see Fig. 5.4.4). On the contrary, the generalized diffusion equation using Laplace and Factorial transformed operators always produce normal diffusive processes. When $1 < s < 3$, however, the time evolution is superdiffusive with the superdiffusive exponent being $\kappa = \frac{2}{s-1}$, which leads to arbitrary values for κ in $(1, \infty)$. Furthermore, we obtained the same supperdiffusive behaviour for the fractional power of the standard Laplacian for large t. However, for small t the behaviour is different.

Chapter 6

Superdiffusive processes on two-dimensional lattice

6.1 Introduction

In the previous chapter a new theoretical framework to study superdiffusive processes on graphs was presented, adding new values to the already existing ones for modelling anomalous diffusion. The main purpose of this chapter is to investigate the existence of superdiffusion in the process termed the *Abstract Cauchy Problem* with the operator that will be given by the transformed k-path LOs defined on an infinite square lattice.

Square lattices are ubiquitous in many real-world physical systems. They are frequently used to describe the spin-1/2 antiferromagnetic Heisenberg model in a number of materials [76, 50, 5, 30]. They are also the preferred model for two-dimensional (2D) gases and optical lattices [13, 54, 48, 1, 73]. Recently, square lattices of superconducting qubits have been employed for error correcting codes in quantum computers [27]. The experimental finding that the native architecture of certain photosynthetic membranes has square lattice shapes [126, 6, 29] is also very significant. This finding is highly relevant in our current work, as the

existence of long-range interactions (LRI) is well documented for light-harvesting complexes. Light harvesting complex or antenna molecules is a pigment-protein complex that are used by plants and photosynthetic bacteria to collect more of the incoming light and transfer it to the reaction centres for the photo-induced redox processes [47, 20, 21]. There is plentiful documentation of the existence of LRI like the ones mathematically described by the k-path LOs considered here for other systems previously mentioned here, such as cold atomic clouds, helium Rydberg atoms and cold Rydberg gases [2, 56, 129]. It is also worthy of note that anomalous diffusion has been observed for ultracold atoms in 2D and 3D lattices [118]. Consequently, the study of a generalised diffusion model on square lattices and proving the conditions for which superdiffusive behaviour exists on them is of considerable theoretical importance because of the many physical processes involved. The contents of this chapter is based on our published work [39].

The structure of the chapter is as follows: in Section 6.2 the solution of the generalised diffusion equation is studied and an integral representation is provided (Theorem 6.3). Then, in Section 6.3 we investigate the asymptotic behaviour of the solution as time tends to infinity. In particular, we formulate and prove the main result (Theorem 6.10). Finally, the behaviour of finite truncations of the Mellin transforms is investigated. Although normal diffusion is present in this case, the coefficient in the diffusion speed can be increased at will if $s \in (2, 4)$ and N is large enough; see Remark 6.12.

6.2 Existence and time evolution of the Mellin transform of the k-path Laplacian on the square lattice

We consider the square lattice, i.e. the graph $\Gamma = P_\infty \times P_\infty = (V, E)$ with vertices $V = \mathbb{Z}^2$ and edges connecting vertices (i, j) and (m, n) when $|i-m| + |j-n| = 1$. We usually write $(u_{x,y})_{x,y\in\mathbb{Z}}$ for functions on V.

We can define a k-path Laplacian on a square lattice as an operator $L_k : \ell^2(V) \to \ell^2(V)$ such that for all $u \in \ell^2(V)$ it takes the form

$$(L_k u)_{x,y} = 4k u_{x,y} - \sum_{j=0}^{k-1} \Big[u_{x+k-j,y+j} + u_{x-k+j,y-j} + u_{x-j,y+k-j} + u_{x+j,y-k+j} \Big],\ x, y \in \mathbb{Z}.$$

Let us consider now an *Abstract Cauchy Problem*

$$u'(t) = -Lu(t); \quad u(0) = \mathring{u}, \tag{6.2.1}$$

with the operator L being the k-path Laplacian L_k or a Mellin-transformed k-path Laplacian operator on a square lattice in the similar way to the infinite path graph which defined in chapter 5.

Using Theorem 4.13 we conclude that $L_{M,s}$ is a well-defined, bounded, self-adjoint and non-negative operator. Again, it allows to describe a process where the particle can jump an arbitrary number of edges with a probability that depends on the length of a jump.

For $m, n \in \mathbb{Z}$ let $\sigma_{m,n} : \ell^2(V) \to \ell^2(V)$ be the shift operator defined by

$$(\sigma_{m,n} u)_{x,y} = u_{x+m,y+n}, \qquad x, y \in \mathbb{Z}.$$

Then L_k can be written as

$$L_k = 4kI - \sum_{j=0}^{k-1} \big[\sigma_{k-j,j} + \sigma_{-k+j,-j} + \sigma_{-j,k-j} + \sigma_{j,-k+j}\big]. \tag{6.2.2}$$

The operator L_k is self-adjoint, so from the spectral theorem we can find a unitary equivalent operator that transforms it into a multiplication operator.

Let us consider the following Fourier transform, which is a unitary operator that is defined by

$$\begin{aligned} &\mathcal{F} : \ell^2(V) \to L^2\big([-\pi,\pi]^2\big), \\ &(\mathcal{F}u)(p,q) = \frac{1}{2\pi} \sum_{x,y\in\mathbb{Z}} u_{x,y} e^{ipx} e^{iqy}, \qquad p,q \in [-\pi,\pi],\ u \in \ell^2(V), \end{aligned}$$

and whose inverse given by

$$(\mathcal{F}^{-1}f)_{x,y} = \frac{1}{2\pi} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} f(p,q) e^{-ipx} e^{-iqy} dp\, dq, \qquad x,y \in \mathbb{Z},\ f \in L^2\big([-\pi,\pi]^2\big).$$

Note, these equations are similar to the Fourier transform that is mentioned in Chapter 5 but here is more complicated.

Now, since

$$\begin{aligned} (\mathcal{F}\sigma_{m,n}u)(p,q) &= \frac{1}{2\pi} \sum_{x,y\in\mathbb{Z}} u_{x+m,y+n} e^{ipx} e^{iqy} = \frac{1}{2\pi} \sum_{x,y\in\mathbb{Z}} u_{x,y} e^{ip(x-m)} e^{iq(y-n)} \\ &= e^{-ipm} e^{-iqn} (\mathcal{F}u)(p,q), \end{aligned}$$

we have

$$\big(\mathcal{F}\sigma_{m,n}\mathcal{F}^{-1}f\big)(p,q) = e^{-i(pm+qn)} f(p,q), \quad p,q \in [-\pi,\pi],\ f \in L^2\big([-\pi,\pi]^2\big). \tag{6.2.3}$$

Together with (6.2.2) we obtain that L_k is unitarily equivalent to a multiplication

operator; more precisely, the following lemma is true.

Lemma 6.1. *With the notations from above we have*

$$\big(\mathcal{F}L_k\mathcal{F}^{-1}f\big)(p,q) = l_k(p,q)f(p,q), \qquad p,q\in[-\pi,\pi],\ f\in L^2\big([-\pi,\pi]^2\big), \tag{6.2.4}$$

where

$$l_k(p,q) = \begin{cases} 4k - i\dfrac{\sin p\cdot\big(e^{ikp}-e^{-ikp}\big)-\sin q\cdot\big(e^{ikq}-e^{-ikq}\big)}{\cos p-\cos q}, & |p|\neq|q|,\\[2ex] 4k + i\cot p\cdot\big(e^{ikp}-e^{-ikp}\big) - k\big(e^{ikp}+e^{-ikp}\big), & |p|=|q|\neq 0,\pi,\\[2ex] 0, & p=q=0,\\[2ex] 4k\big(1-(-1)^k\big), & |p|=|q|=\pi. \end{cases}$$

Moreover, l_k is continuous and even in both p and q, and the following inequalities hold:

$$0\le l_k(p,q)\le 8k, \qquad p,q\in[-\pi,\pi], \tag{6.2.5}$$

$$l_1(p,q)>0, \qquad (p,q)\in[-\pi,\pi]^2\setminus\{(0,0)\}. \tag{6.2.6}$$

Proof. It follows from (6.2.2) and (6.2.3) that (6.2.4) holds with

$$\begin{aligned} l_k(p,q) &= 4k - \sum_{j=0}^{k-1}\Big[e^{-i[(k-j)p+jq]} - e^{-i[(-k+j)p-jq]} \\ &\qquad\qquad - e^{-i[-jp+(k-j)q]} - e^{-i[jp+(-k+j)q]}\Big] \\ &= 4k - e^{-ikp}\sum_{j=0}^{k-1}e^{ij(p-q)} + e^{ikp}\sum_{j=0}^{k-1}e^{-ij(p-q)} \\ &\quad + e^{-ikq}\sum_{j=0}^{k-1}e^{ij(p+q)} + e^{ikq}\sum_{j=0}^{k-1}e^{-ij(p+q)}. \end{aligned} \tag{6.2.7}$$

When $|p| \neq |q|$ we can rewrite this as follows:

$$\begin{aligned} l_k(p,q) &= 4k - \frac{e^{-ikp} - e^{-ikq}}{1 - e^{i(p-q)}} - \frac{e^{ikp} - e^{ikq}}{1 - e^{-i(p-q)}} - \frac{e^{-ikq} - e^{ikp}}{1 - e^{i(p+q)}} - \frac{e^{ikq} - e^{-ikp}}{1 - e^{-i(p+q)}} \\ &= 4k - e^{ikp}\left(\frac{1}{1 - e^{-ip+iq}} - \frac{1}{1 - e^{ip+iq}}\right) - e^{-ikp}\left(\frac{1}{1 - e^{ip-iq}} - \frac{1}{1 - e^{-ip-iq}}\right) \\ &\quad + e^{ikq}\left(\frac{1}{1 - e^{-ip+iq}} - \frac{1}{1 - e^{-ip-iq}}\right) + e^{-ikq}\left(\frac{1}{1 - e^{ip-iq}} - \frac{1}{1 - e^{ip+iq}}\right). \end{aligned}$$

The expressions within the brackets can be simplified, e.g.

$$\begin{aligned} &\frac{1}{1 - e^{-ip+iq}} - \frac{1}{1 - e^{ip+iq}} = \frac{e^{-ip+iq} - e^{ip+iq}}{1 - e^{-ip+iq} - e^{ip+iq} + e^{2iq}} \\ &= \frac{e^{-ip} - e^{ip}}{e^{-iq} - e^{-ip} - e^{ip} + e^{iq}} = \frac{i \sin p}{\cos p - \cos q}. \end{aligned}$$

Hence

$$\begin{aligned} l_k(p,q) &= 4k - e^{ikp}\frac{i \sin p}{\cos p - \cos q} + e^{-ikp}\frac{i \sin p}{\cos p - \cos q} \\ &\quad + e^{ikq}\frac{i \sin q}{\cos p - \cos q} - e^{-ikq}\frac{i \sin q}{\cos p - \cos q} \\ &= 4k - \frac{i}{\cos p - \cos q}\Big[\sin p \cdot \left(e^{ikp} - e^{-ikp}\right) - \sin q \cdot \left(e^{ikq} - e^{-ikq}\right)\Big]. \end{aligned}$$

For the case when $|p| = |q|$ note that l_k is continuous by (6.2.7). Write l_k as

$$l_k(p,q) = 4k - i\frac{f(p) - f(q)}{g(p) - g(q)},$$

with $f(p) = \sin p \cdot (e^{ikp} - e^{-ikp})$ and $g(p) = \cos p$. The Generalized Mean Value Theorem implies that

$$l_k(p,q) = 4k - i\frac{f'(\xi)}{g'(\xi)},$$

with ξ between p and q. Hence

$$\begin{aligned} l_k(p,p) &= \lim_{q\to p} l_k(p,q) = 4k - i\frac{f'(p)}{g'(p)} \\ &= 4k - i\frac{\cos p\cdot(e^{ikp}-e^{-ikp}) + ik\sin p\cdot(e^{ikp}+e^{-ikp})}{-\sin p} \\ &= 4k + i\cot p\cdot\big(e^{ikp}-e^{-ikp}\big) - k\big(e^{ikp}+e^{-ikp}\big). \end{aligned} \tag{6.2.8}$$

The relation $l_k(0,0) = 0$ follows from (6.2.7), and the value for $l_k(p,q)$ when $|p| = |q| = \pi$ follows from (6.2.8) by taking the limit $p \to \pi$. That l_k is even in p and q is clear. Since L_k is a non-negative operator in $\ell^2(V)$ as describe in Chapter 4, Section 2, the function l_k is non-negative. The upper bound for l_k in (6.2.5) follows from (6.2.7).

Finally, to show (6.2.6) rewrite l_1; for $|p| \neq |q|$ we have

$$l_1(p,q) = 4 + 2\frac{\sin^2 p - \sin^2 q}{\cos p - \cos q} = 4 - 2(\cos p + \cos q), \tag{6.2.9}$$

which extends to all $p, q \in [-\pi,\pi]$ by continuity. The right-hand side of (6.2.9) is strictly positive unless $p = q = 0$. □

Let us now consider the Mellin transformation of the k-path Laplacians L_k, i.e. the operator

$$L_{M,s} = \sum_{k=1}^{\infty} \frac{1}{k^s} L_k. \tag{6.2.10}$$

Since $\|L_k\| \leq 8k$ by Lemma (6.1), the series converges in the operator norm when $s > 2$. As the next lemma shows, the operator $L_{M,s}$ is also unitarily equivalent to a multiplication operator in $L^2([-\pi,\pi]^2)$.

Lemma 6.2. *For $s > 2$ we have*

$$\big(\mathcal{F}L_{M,s}s\mathcal{F}^{-1}f\big)(p,q) = l_{M,s}(p,q)f(p,q), \quad p,q\in[-\pi,\pi],\ f\in L^2\big([-\pi,\pi]^2\big), \tag{6.2.11}$$

where

$$l_{M,s}(p,q) := \sum_{k=1}^{\infty} \frac{1}{k^s}\, l_k(p,q), \tag{6.2.12}$$

$$= \begin{cases} 4\zeta(s-1) + \dfrac{g_s(p) - g_s(q)}{\cos p - \cos q}\,, & |p| \neq |q|, \\ 4\zeta(s-1) - 2\cot p \cdot Im\big(Li_s(e^{ip})\big) - 2Re\big(Li_{s-1}(e^{ip})\big), & |p| = |q| \neq 0, \pi, \\ 0, & p = q = 0, \\ 4\big(1-(-1)^k\big)\zeta(s-1), & |p| = |q| = \pi, \end{cases}$$

where Li_s is the polylogarithm function which defined in (1.8.1) *and*

$$g_s(p) := 2\sin p \cdot Im\big(Li_s(e^{ip})\big). \tag{6.2.13}$$

The function $l_{M,s}$ is continuous and even in both p and q, and the following inequalities hold:

$$0 \leq l_{M,s}(p,q) \leq 8\zeta(s-1), \qquad p,q \in [-\pi,\pi], \tag{6.2.14}$$

$$l_{M,s}(p,q) > 0, \qquad (p,q) \in [-\pi,\pi]^2 \setminus \{(0,0)\}. \tag{6.2.15}$$

Proof. It follows from Lemma 6.1 that (6.2.11) holds with $l_{m,s}$ defined as in (6.2.12). When $|p| \neq |q|$, we have

$$l_{M,s}(p,q) = \sum_{k=1}^{\infty} \frac{1}{k^s}\left[4k - i\frac{\sin p \cdot \big(e^{ikp} - e^{-ikp}\big) - \sin q \cdot \big(e^{ikq} - e^{-ikq}\big)}{\cos p - \cos q}\right]$$

$$
\begin{aligned}
l_{M,s}(p,q) &= 4\sum_{k=1}^{\infty}\frac{1}{k^{s-1}} - \frac{i}{\cos p-\cos q}\Big[\sin p\cdot\sum_{k=1}^{\infty}\frac{1}{k^s}\Big((e^{ip})^k-(e^{-ip})^k\Big)\\
&\quad -\sin q\cdot\sum_{k=1}^{\infty}\frac{1}{k^s}\Big((e^{iq})^k-(e^{-iq})^k\Big)\Big]\\
&= 4\zeta(s-1) - \frac{i}{\cos p-\cos q}\Big[\sin p\cdot\Big(Li_s(e^{ip})-Li_s(e^{-ip})\Big)\\
&\quad -\sin q\cdot\Big(Li_s(e^{iq})-Li_s(e^{-iq})\Big)\Big],
\end{aligned}
$$

which proves the formula for $l_{M,s}$ in the first case. Now assume that $|p|=|q|\neq 0,\pi$. Then

$$
\begin{aligned}
l_{M,s}(p,q) &= \sum_{k=1}^{\infty}\frac{1}{k^s}\Big[4k + i\cot p\cdot\big(e^{ikp}-e^{-ikp}\big) - k\big(e^{ikp}+e^{-ikp}\big)\Big]\\
&= 4\sum_{k=1}^{\infty}\frac{1}{k^{s-1}} + i\cot p\cdot\sum_{k=1}^{\infty}\frac{1}{k^s}\Big((e^{ip})^k-(e^{-ip})^k\Big) - \sum_{k=1}^{\infty}\frac{1}{k^{s-1}}\Big((e^{ip})^k+(e^{-ip})^k\Big)\\
&= 4\zeta(s-1) + i\cot p\cdot\big(Li_s(e^{ip})-Li_s(e^{-ip})\big) - Li_{s-1}(e^{ip}) - Li_{s-1}(e^{-ip}).
\end{aligned}
$$

The remaining cases are clear. The continuity of $l_{M,s}$ follows from the continuity of l_k and the fact that the series in (6.2.12) converges uniformly. The symmetry of $l_{M,s}$ and the inequalities in (6.2.14) follows directly from the symmetry of l_k and (6.2.5). The inequality in (6.2.15) follows from (6.2.6) and the first inequality in (6.2.5). □

Since $L_{M,s}$ is a bounded operator, the Cauchy problem

$$
\frac{d}{dt}u(t) = -L_{M,s}u(t), \qquad t>0, \tag{6.2.16}
$$

$$
u(0) = \mathring{u}, \tag{6.2.17}
$$

has a unique solution, which is given by

$$u(t) = e^{-tL_{M,s}}\mathring{u}, \qquad t \geq 0.$$

It follows from Lemma 6.2 that

$$\big(\mathcal{F}e\mathcal{F}^{-1}f\big)(p,q) = e^{-tl_{M,s}(p,q)}f(p,q),\ t \geq 0,\ p,q \in [-\pi,\pi],\ f \in L^2\big([-\pi,\pi]^2\big). \tag{6.2.18}$$

Using this relation and the fact that $l_{M,s}$ is even one can easily show the following theorem; cf. Theorem 5.3 for the case of the infinite path graph. For the formulation of the theorem let $e_{m,n} \in \ell^2(V)$ be the vector defined by

$$(e_{m,n})_{x,y} = \begin{cases} 1, & m = x,\ n = y, \\ 0, & \text{otherwise.} \end{cases} \tag{6.2.19}$$

Theorem 6.3. *Let $s > 2$ and $\mathring{u} \in \ell^2(V)$. The unique solution of* (6.2.16), (6.2.17) *is given by*

$$u_{x,y}(t) = \frac{1}{4\pi^2}\sum_{m,n\in\mathbb{Z}} \mathring{u} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} e^{i[(x-m)p+(y-n)q]}e^{-tl_{M,s}(p,q)}dp\,dq, \qquad x,y \in \mathbb{Z}.$$

In particular, for $\mathring{u} = e_{0,0}$ we obtain

$$u_{x,y}(t) = \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} e^{i(xp+yq)}e^{-tl_{M,s}(p,q)}dp\,dq, \qquad x,y \in \mathbb{Z}. \tag{6.2.20}$$

Proof. In order to find a semigroup solution of a form $u(t) = e^{-tL_{M,s}}\mathring{u}$ for $t \geq 0$. Firstly, note that $l_{M,s}(x,y)$ is an even function according to both coordinates. Using the formulas for Fourier series and inverse Fourier series, the definition of

base in $\ell^2(V)$ and the fact that function $l_{M,s}$ is even, we have

$$\begin{aligned}\left(e^{-tL_{M,s}}e_{mn}\right)_{xy} &= \left(\mathcal{F}^{-1}e^{-tl_{M,s}(\cdot,\cdot)}\mathcal{F}e_{mn}\right)_{xy} \\ &= \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} e^{-ixp}e^{-iyq}e^{-tl_{M,s}(p,q)}\sum_{j\in\mathbb{Z}}\sum_{s\in\mathbb{Z}} e_{vw}e^{ijp}e^{isq}dpdq \\ &= \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} e^{i(x-m)p}e^{i(y-n)q}e^{-tl_{M,s}(p,q)}dxdy.\end{aligned}$$

Represent an initial condition $\mathring{u} = (\mathring{u}_{pq})_{p,q\in\mathbb{Z}}$ as a linear combination of elements from the base $\mathring{u} = \sum_{p,q\in\mathbb{Z}} \mathring{u}e_{pq}$ the solution takes the form

$$e^{-tL_{M,s}}\mathring{u} = \sum_{p,q\in\mathbb{Z}} e^{-tL_{M,s}}e_{pq}\mathring{u}.$$

Note that because of the boundedness of the operators $e^{-tL_{M,s}}$ for any $t \in (0,\infty)$, the solution is well defined and takes the form

$$u(t)_{xy} = \frac{1}{4\pi^2}\sum_{m\in\mathbb{Z}}\sum_{n\in\mathbb{Z}}\mathring{u}_{vw}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} e^{i(x-m)p}e^{i(y-n)q}e^{-tl_{M,s}(p,q)}dpdq.$$

Especially for initial condition $\mathring{u}(x,y) = e_{00}$, using a symmetry of integrand function we obtain

$$e^{-tL_{M,s}}e_{xy,00} = \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\cos(xp)\cos(yq)e^{-tl_{M,s}(p,q)}dpdq.$$

□

6.3 Diffusion and superdiffusion for the Mellin transformed k-path Laplacian on a square lattice

In this section we examine the long-time behaviour of the solution to the Cauchy problem generated by the Mellin-transformed k-path Laplacian. The main result is contained in Theorem 6.10. To prove this theorem we first examine the asymptotic behaviour of the function $l_{M,s}$ (see Fig. 6.3.1) as the arguments tend to zero, which is contained in Proposition 6.8. The discussion is based on similar considerations undertaken for the path graph in the previous chapter, but the arguments are more subtle. We start with a simple lemma, which is used a couple of times below.

Lemma 6.4. *Let $b > 0$, let $f : (0, b) \to \mathbb{R}$ be differentiable and assume that*

$$|f'(t)| \leq Ct^{\alpha}, \qquad t \in (0, b),$$

for some $C > 0$ and $\alpha \geq 1$. Then

$$\left| \frac{f(p) - f(q)}{p^2 - q^2} \right| \leq \frac{C}{2} \max\{p^{\alpha-1}, q^{\alpha-1}\}, \qquad p, q \in (0, b),\ p \neq q.$$

Proof. Define the function $g(x) := f(\sqrt{x})$, $x \in (0, b^2)$. Let $p, q \in (0, b)$ such that $p \neq q$ and set $x := p^2$, $y := q^2$. Then

$$\left| \frac{f(p) - f(q)}{p^2 - q^2} \right| = \left| \frac{g(x) - g(y)}{x - y} \right| = |g'(\xi)|, \tag{6.3.1}$$

for some ξ between x and y by the Mean Value Theorem. Since $\sqrt{\xi} \leq \max\{p, q\}$,

we obtain that

$$|g'(\xi)| = \left|\frac{f'(\sqrt{\xi})}{2\sqrt{\xi}}\right| \le \frac{C(\sqrt{\xi})^{\alpha}}{2\sqrt{\xi}} \le \frac{C}{2}\max\{p^{\alpha-1}, q^{\alpha-1}\},$$

which, together with (6.3.1), finishes the proof. □

In the next three lemmas we prove auxiliary asymptotic results, which are used to obtain the asymptotic behaviour of $l_{M,s}$ in Proposition 6.8.

Lemma 6.5. *We have*

$$\frac{1}{\cos p - \cos q} = -\frac{2}{p^2 - q^2}\left[1 + \frac{1}{12}\big(p^2 + q^2\big) + R_1(p,q)\right], \quad p, q \in [-\pi, \pi],\ |p| \neq |q|.$$

where

$$R_1(p,q) = O\big(p^4 + q^4\big), \qquad p, q \to 0,\ |p| \neq |q|.$$

Proof. We write

$$\cos p = 1 - \frac{p^2}{2} + \frac{p^4}{24} + f(p),$$

where $f'(p) = O(p^5)$, $p \to 0$. For $p, q \in (0, \pi]$ with $|p| \neq |q|$ we have

$$\begin{aligned}
\cos p - \cos q &= -\frac{p^2 - q^2}{2} + \frac{p^4 - q^4}{24} + f(p) - f(q) \\
&= -\frac{1}{2}(p^2 - q^2)\left[1 - \frac{1}{12}\big(p^2 + q^2\big) - 2\frac{f(p) - f(q)}{p^2 - q^2}\right] \\
&= -\frac{1}{2}(p^2 - q^2)\left[1 - \frac{1}{12}\big(p^2 + q^2\big) + O\big(p^4 + q^4\big)\right], \qquad p, q \to 0,
\end{aligned}$$

where the last relation follows from Lemma 6.4. Now the claim is obtained by taking inverses on both sides and extending the result to non-positive p, q by continuity and symmetry. □

Lemma 6.6. *Let $s \in (2, \infty) \setminus \{4\}$. Then*

$$2\mathrm{Im}\big(Li_s(e^{ip})\big) = -\frac{C_s}{2}p^{s-1} + 2\zeta(s-1)p - \frac{\zeta(s-3)}{3}p^3 + R_{2,s}(p), \qquad p \in (0, 2\pi),$$

where

$$C_s := \begin{cases} -\dfrac{2\pi}{\Gamma(s)\sin(\frac{s\pi}{2})}, & s \notin 2\mathbb{Z}, \\ 0, & s \in 2\mathbb{Z}, \end{cases} \tag{6.3.2}$$

and

$$R_{2,s}(p) = O(p^5) \quad \textit{and} \quad R'_{2,s}(p) = O(p^4), \qquad p \searrow 0, \qquad \textit{if } s \neq 6,$$

and

$$R_{2,s}(p) = O\big(p^5|\ln p|\big) \quad \textit{and} \quad R'_{2,s}(p) = O\big(p^4|\ln p|\big), \qquad p \searrow 0, \qquad \textit{if } s = 6.$$

Proof. First let $s \in (2,\infty) \setminus \mathbb{N}$. It follows from (1.8.3) that, for $p \in (0, 2\pi)$,

$$\begin{aligned} 2\mathrm{Im}\big(Li_s(e^{ip})\big) &= 2\mathrm{Im}\left[\Gamma(1-s)(-ip)^{s-1} + \sum_{n=0}^{\infty}\zeta(s-n)\frac{(ip)^n}{n!}\right] \\ &= 2\mathrm{Im}\left[\Gamma(1-s)p^{s-1}e^{-(s-1)\frac{\pi}{2}i} + \sum_{n=0}^{\infty}\zeta(s-n)\frac{i^n p^n}{n!}\right] \\ &= -2\Gamma(1-s)\sin\Big((s-1)\frac{\pi}{2}\Big)p^{s-1} + 2\sum_{l=0}^{\infty}\zeta(s-2l-1)\frac{(-1)^l}{(2l+1)!}p^{2l+1} \\ &= -\frac{C_s}{2}p^{s-1} + 2\zeta(s-1)p - \frac{\zeta(s-3)}{3}p^3 + R_{2,s}(p), \end{aligned}$$

where

$$\begin{aligned} C_s &= 4\Gamma(1-s)\sin\Big((s-1)\frac{\pi}{2}\Big) = \frac{4\pi\sin\big((s-1)\frac{\pi}{2}\big)}{\Gamma(s)\sin(s\pi)} = -\frac{4\pi\cos(\frac{s\pi}{2})}{\Gamma(s)\sin(s\pi)} \\ &= -\frac{2\pi}{\Gamma(s)\sin(\frac{s\pi}{2})}, \end{aligned}$$

and

$$R_{2,s}(p) = 2\sum_{l=2}^{\infty}\zeta(s-2l-1)\frac{(-1)^l}{(2l+1)!}p^{2l+1}.$$

This relation extends to s being an odd integer with $s \geq 3$. Moreover, $R_{2,s}$ satisfies

$$R_{2,s}(p) = O(p^5) \quad \text{and} \quad R'_{2,s}(p) = O(p^4), \qquad p \searrow 0.$$

This proves the claim for $s \in (2, \infty) \setminus 2\mathbb{N}$.

Now let $s \in \{6, 8, \ldots\}$ and set

$$H_n = \sum_{j=1}^{n} \frac{1}{j}\,.$$

From (1.8.4) we obtain, again for $p \in (0, 2\pi)$,

$$\begin{aligned}
2\mathrm{Im}\big(Li_s(e^{ip})\big) &= 2\mathrm{Im}\left[\frac{(ip)^{s-1}}{(s-1)!}\Big(H_{s-1} - \log(-ip)\Big) + \sum_{\substack{n=0\\ n\neq s-1}}^{\infty} \zeta(s-n)\frac{(ip)^n}{n!}\right] \\
&= 2\mathrm{Im}\left[\frac{(-1)^{\frac{s}{2}-1} i p^{s-1}}{(s-1)!}\Big(H_{s-1} - \ln p + i\frac{\pi}{2}\Big) + \sum_{\substack{n=0\\ n\neq s-1}}^{\infty} \zeta(s-n)\frac{i^n p^n}{n!}\right] \\
&= \frac{2(-1)^{\frac{s}{2}-1}}{(s-1)!} p^{s-1}\big(H_{s-1} - \ln p\big) + 2 \sum_{\substack{l=0\\ l\neq \frac{s}{2}-1}}^{\infty} \zeta(s-2l-1)\frac{(-1)^l}{(2l+1)!} p^{2l+1} \\
&= 2\zeta(s-1)p - \frac{\zeta(s-3)}{3}p^3 + R_{2,s}(p),
\end{aligned}$$

where

$$R_{2,s}(p) = \frac{2(-1)^{\frac{s}{2}-1}}{(s-1)!} p^{s-1}\big(H_{s-1} - \ln p\big) + 2 \sum_{\substack{l=2\\ l\neq \frac{s}{2}-1}} \zeta(s-2l-1)\frac{(-1)^l}{(2l+1)!} p^{2l+1},$$

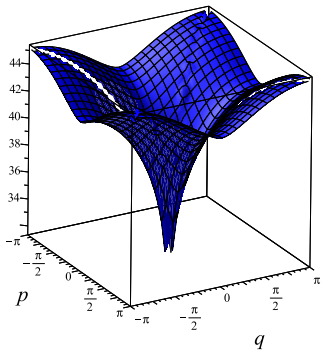
which satisfies

$$R_{2,s}(p) = O(p^5) \quad \text{and} \quad R'_{2,s}(p) = O(p^4), \qquad p \searrow 0, \qquad \text{if } \ s \geq 8,$$

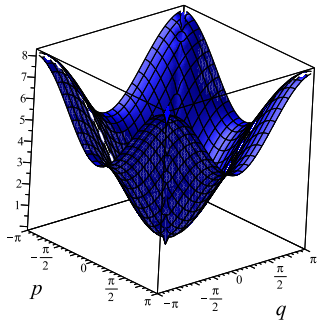
and

$$R_{2,s}(p) = O\big(p^5|\ln p|\big) \quad \text{and} \quad R'_{2,s}(p) = O\big(p^4|\ln p|\big), \qquad p \searrow 0, \qquad \text{if } s = 6.$$

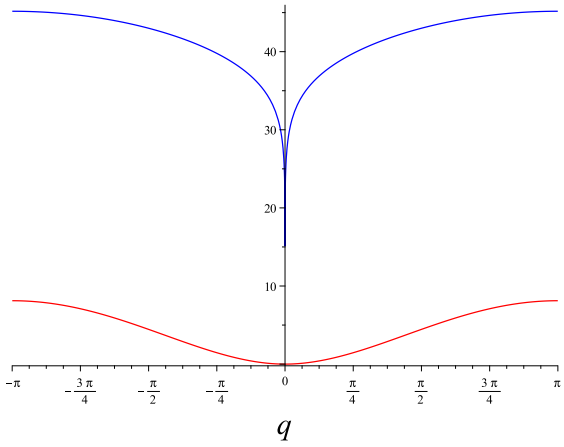
This finishes the proof in the case when $s \in \{6, 8, \ldots\}$. □



(a) $s = 2.1$



(b) $s = 5$



(c) $l_{M,s}$ restricted to $p = q$ for $s = 2.1$ (blue) and $s = 5$ (red), respectively

Figure 6.3.1: The graph of the function $l_{M,s}$ on the square $[-\pi, \pi]^2$ for the parameters $s = 2.1$ (a) and $s = 5$ (b), respectively. The third graph (c) shows the behaviour of both solutions $s = 2.1$ and $s = 5$ restricted to the line $p = q$.

Lemma 6.7. *Let $s \in (2, \infty) \setminus \{4\}$ and let g_s be defined as in* (6.2.13) *and C_s as in* (6.3.2). *Then*

$$g_s(p) = -\frac{C_s}{2}p^s + 2\zeta(s-1)p^2 - \frac{\zeta(s-1) + \zeta(s-3)}{3}p^4 + R_{3,s}(p),$$

where $R_{3,s}$ satisfies

$$R'_{3,s}(p) = \begin{cases} O(p^{s+1}), & s \in (2,4), \\ O(p^5), & s \in (4,\infty) \setminus \{6\}, \\ O\big(p^5 |\ln p|\big), & s = 6, \end{cases} \tag{6.3.3}$$

as $p \searrow 0$.

Proof. Write $\sin p = p - \frac{p^3}{6} + R_{sin}(p)$. From Lemma 6.6 we obtain that

$$\begin{aligned} g_s(p) &= 2 \sin p \cdot \mathrm{Im}\big(Li_s(e^{ip})\big) \\ &= \left[p - \frac{p^3}{6} + R_{sin}(p)\right]\left[-\frac{C_s}{2}p^{s-1} + 2\zeta(s-1)p - \frac{\zeta(s-3)}{3}p^3 + R_{2,s}(p)\right] \\ &= -\frac{C_s}{2}p^s + 2\zeta(s-1)p^2 - \frac{\zeta(s-1)+\zeta(s-3)}{3}p^4 + R_{3,s}(p), \end{aligned}$$

where

$$\begin{aligned} R_{3,s}(p) = \frac{C_s}{12}p^{s+2} - \frac{C_s}{2}p^{s-1}R_{sin}(p) + 2\zeta(s-1)pR_{sin}(p) \\ + \frac{\zeta(s-3)}{18}p^6 - \frac{\zeta(s-3)}{3}p^3 R_{sin}(p) + \sin p \cdot R_{2,s}(p), \end{aligned}$$

which satisfies

$$R'_{3,s}(p) = O(p^{s+1}) + O(p^5) + O\big(R_{2,s}(p)\big) + O\big(pR'_{2,s}(p)\big).$$

The latter relation yields (6.3.3). □

In the next proposition we consider the asymptotic behaviour of the function $l_{M,s}$ around the origin. In particular, we observe that the behaviour differs for the two cases $s \in (2,4)$ and $s \in (4,\infty)$. For the case when $s = 4$ the behaviour is more complicated and involves a logarithmic term; we do not consider this case

in the following.

Proposition 6.8. *Let $s \in (2,\infty) \setminus \{4\}$, let $l_{M,s}$ be as in (6.2.12) and C_s as in (6.3.2). Moreover, define*

$$h_{1,s}(p,q) := \begin{cases} C_s \dfrac{|p|^s - |q|^s}{p^2 - q^2}, & |p| \neq |q|, \\ \dfrac{sC_s}{2}|p|^{s-2}, & |p| = |q|, \end{cases}$$

$$h_{2,s}(p,q) := \frac{\zeta(s-1) + 2\zeta(s-3)}{3}(p^2 + q^2).$$

Then

$$l_{M,s}(p,q) = h_{1,s}(p,q) + h_{2,s}(p,q) + R_s(p,q), \qquad p,q \in [-\pi,\pi],$$

where

$$R_s(p,q) = O\big(p^\alpha + q^\alpha\big), \qquad p,q \to 0,$$

with

$$\alpha = \begin{cases} \min\{s,4\}, & s \neq 6, \\ 4-\epsilon, & s = 6, \end{cases}$$

with an arbitrary $\epsilon > 0$.

In particular, we have

$$l_{M,s}(p,q) = \begin{cases} h_{1,s}(p,q) + O(p^s + q^s), & s \in (2,4), \\ h_{2,s}(p,q) + O(p^4 + q^4), & s \in (4,\infty) \setminus \{6\}, \\ h_{2,s}(p,q) + O(p^{4-\epsilon} + q^{4-\epsilon}), & s = 6, \end{cases}$$

as $p,q \to 0$ with arbitrary $\epsilon > 0$ when $s = 6$.

Proof. Let $p,q \in (0,\pi]$ such that $|p| \neq |q|$. From Lemmas 6.2, 6.5 and 6.7 we

obtain

$$
\begin{aligned}
l_{M,s}(p,q) &= 4\zeta(s-1) + \frac{g_s(p)-g_s(q)}{\cos p - \cos q} \\
&= 4\zeta(s-1) - \frac{2}{p^2-q^2}\Big[1+\frac{1}{12}\big(p^2+q^2\big)+R_1(p,q)\Big]\times \\
&\quad\times\Big[-\frac{C_s}{2}(p^s-q^s)+2\zeta(s-1)(p^2-q^2)-\frac{\zeta(s-1)+\zeta(s-3)}{3}\big(p^4-q^4\big) \\
&\qquad + R_{3,s}(p)-R_{3,s}(q)\Big] \\
&= 4\zeta(s-1)+\Big[1+\frac{1}{12}\big(p^2+q^2\big)+R_1(p,q)\Big]\cdot\Big[C_s\frac{p^s-q^s}{p^2-q^2} \\
&\quad - 4\zeta(s-1)+\frac{2}{3}\Big(\zeta(s-1)+\zeta(s-3)\Big)(p^2+q^2)-2\frac{R_{3,s}(p)-R_{3,s}(q)}{p^2-q^2}\Big] \\
&= C_s\frac{p^s-q^s}{p^2-q^2}+\Big[\frac{2}{3}\Big(\zeta(s-1)+\zeta(s-3)\Big)-\frac{1}{3}\zeta(s-1)\Big](p^2+q^2)+R_s(p,q),
\end{aligned}
$$

where

$$
\begin{aligned}
R_s(p,q) = C_s&\Big[\frac{1}{12}\big(p^2+q^2\big)+R_1(p,q)\Big]\frac{p^s-q^s}{p^2-q^2} \\
&+R_1(p,q)\Big[-4\zeta(s-1)+\frac{2}{3}\Big(\zeta(s-1)+\zeta(s-3)\Big)(p^2+q^2)\Big] \\
&+\frac{1}{18}\Big(\zeta(s-1)+\zeta(s-3)\Big)(p^2+q^2)^2 \\
&-2\Big[1+\frac{1}{12}\big(p^2+q^2\big)+R_1(p,q)\Big]\frac{R_{3,s}(p)-R_{3,s}(q)}{p^2-q^2}\,.
\end{aligned}
$$

It follows from Lemma 6.7 that

$$
R'_{3,s}(p)=O(p^\beta)\qquad \text{where } \beta=\begin{cases}\min\{s+1,5\}, & s\neq 6,\\ 5-\epsilon, & s=6,\end{cases} \tag{6.3.4}
$$

for arbitrary $\epsilon > 0$. Lemma 6.4 implies that

$$\frac{p^s - q^s}{p^2 - q^2} = O\big(p^{s-2} + q^{s-2}\big), \qquad q, p \to 0,\ p \neq q,$$

and

$$\frac{R_{3,s}(p) - R_{3,s}(q)}{p^2 - q^2} = O(p^{\beta-1}), \qquad q, p \to 0,\ p \neq q,$$

where β is as in (6.3.4). The error term R_s satisfies

$$R_s(p, q) = O\big(p^\alpha + q^\alpha\big), \qquad p, q \to 0,\ p \neq q,$$

where

$$\alpha = \begin{cases} \min\{s, 4\}, & s \neq 6, \\ 4 - \epsilon, & s = 6, \end{cases}$$

with an arbitrary $\epsilon > 0$. Since $l_{M,s}$, $h_{1,s}$ and $h_{2,s}$ are continuous and even in p and q, the result extends to all $p, q \in [-\pi, \pi]$. □

The next lemma is the key lemma about the long-time behaviour of the solution of the Cauchy problem; it is a generalization of lemma 5.5 to the two-dimensional setting. It is more subtle than the one-dimensional case, but a further generalization to n dimensions is straightforward.

Lemma 6.9. *Let $\alpha > 0$ and let $l : [-\pi, \pi]^2 \to \mathbb{R}$ be a continuous function that satisfies*

$$l(p, q) > 0, \qquad (p, q) \in [-\pi, \pi]^2 \setminus \{(0, 0)\}, \tag{6.3.5}$$

and can be written as

$$l(p, q) = h(p, q) + R(p, q),$$

where the continuous function $h : \mathbb{R}^2 \to \mathbb{R}$ satisfies

$$h(rp, rq) = r^\alpha h(p, q), \qquad r > 0,\ p, q \in \mathbb{R},$$

and

$$R(p,q) = o\big(|p|^\alpha + |q|^\alpha\big), \qquad p,q \to 0. \tag{6.3.6}$$

Define the function

$$f(x,y,t) := \frac{1}{4\pi^2} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} e^{i(xp+yq)} e^{-tl(p,q)}\, dp\, dq, \qquad x,y \in \mathbb{R}.$$

Then

$$t^{\frac{2}{\alpha}} f\big(t^{\frac{1}{\alpha}}\xi, t^{\frac{1}{\alpha}}\eta, t\big) \to \frac{1}{4\pi^2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i(\xi v+\eta w)} e^{-h(v,w)}\, dv\, dw := F(\xi,\eta), \qquad t \to \infty, \tag{6.3.7}$$

uniformly in $\xi, \eta \in \mathbb{R}$.

Hence

$$f(x,y) = t^{-\frac{2}{\alpha}} F\big(t^{-\frac{1}{\alpha}}x, t^{-\frac{1}{\alpha}}y\big) + o\big(t^{-\frac{2}{\alpha}}\big), \qquad t \to \infty, \tag{6.3.8}$$

uniformly in $x, y \in \mathbb{R}$.

Proof. Let us first show that there exists $C > 0$ such that

$$l(p,q) \geq C\big(|p|^\alpha + |q|^\alpha\big), \qquad p,q \in [-\pi,\pi]. \tag{6.3.9}$$

For fixed $(p,q) \in \mathbb{R}^2 \setminus \{(0,0)\}$ we have

$$l(rp,rq) = r^\alpha h(p,q) + o(r^\alpha), \qquad r \searrow 0,$$

which, together with (6.3.5) implies that $h(p,q) > 0$ for $(p,q) \in R^2 \setminus \{(0,0)\}$. Set

$$C_1 := \min_{|p|^\alpha + |q|^\alpha = 1} h(p,q),$$

which is a positive number. Let $(p,q) \in \mathbb{R}^2 \setminus \{(0,0)\}$ and set $r := (|p|^\alpha + |q|^\alpha)^{\frac{1}{\alpha}}$.

Then

$$h(p,q) = h\Big(r\frac{p}{r}, r\frac{q}{r}\Big) = r^\alpha h\Big(\frac{p}{r}, \frac{q}{r}\Big) \geq C_1 r^\alpha$$

and hence

$$h(p,q) \geq C_1\big(|p|^\alpha + |q|^\alpha\big), \qquad p,q \in \mathbb{R}. \tag{6.3.10}$$

Together with (6.3.6), this implies that

$$l(p,q) \geq \frac{C_1}{2}\big(|p|^\alpha + |q|^\alpha\big), \qquad p,q \in \mathbb{R} \text{ such that } |p|^\alpha + |q|^\alpha \leq r_0$$

for some $r_0 > 0$. Since l is continuous and satisfies (6.3.5), we obtain (6.3.9).

For $\xi, \eta \in \mathbb{R}$ and $t > 0$ we can use the substitution $v = t^{\frac{1}{\alpha}}p$, $w = t^{\frac{1}{\alpha}}q$ to obtain

$$\begin{aligned} t^{\frac{2}{\alpha}} f\big(t^{\frac{1}{\alpha}}\xi, t^{\frac{1}{\alpha}}\eta, t\big) &= t^{\frac{2}{\alpha}} \frac{1}{4\pi^2} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} e^{it^{\frac{1}{\alpha}}(\xi p + \eta q)} e^{-tl(p,q)}\, dp\, dq \\ &= \frac{1}{4\pi^2} \int_{-t^{-\frac{1}{\alpha}}\pi}^{t^{-\frac{1}{\alpha}}\pi}\int_{-t^{-\frac{1}{\alpha}}\pi}^{t^{-\frac{1}{\alpha}}\pi} e^{i(\xi v + \eta w)} e^{-tl(t^{-\frac{1}{\alpha}}v, t^{-\frac{1}{\alpha}}w)}\, dv\, dw. \end{aligned}$$

Hence

$$\begin{aligned} &\Big| t^{\frac{2}{\alpha}} f\big(t^{\frac{1}{\alpha}}\xi, t^{\frac{1}{\alpha}}\eta, t\big) - F(\xi,\eta) \Big| \\ &= \Bigg| \frac{1}{4\pi^2} \iint\limits_{[-t^{-\frac{1}{\alpha}}\pi, t^{-\frac{1}{\alpha}}\pi]^2} e^{i(\xi v + \eta w)} \Big(e^{-tl(t^{-\frac{1}{\alpha}}v, t^{-\frac{1}{\alpha}}w)} - e^{-h(v,w)} \Big)\, dv\, dw \\ &\quad - \frac{1}{4\pi^2} \iint\limits_{\mathbb{R}^2 \setminus [-t^{-\frac{1}{\alpha}}\pi, t^{-\frac{1}{\alpha}}\pi]^2} e^{i(\xi v + \eta w)} e^{-h(v,w)}\, dv\, dw \Bigg| \end{aligned}$$

$$\leq \frac{1}{4\pi^2} \iint\limits_{\mathbb{R}^2} \chi_{[-t^{-\frac{1}{\alpha}}\pi, t^{-\frac{1}{\alpha}}\pi]^2}(v,w) \Big| e^{-tl(t^{-\frac{1}{\alpha}}v, t^{-\frac{1}{\alpha}}w)} - e^{-h(v,w)} \Big| \, dv\, dw \tag{6.3.11}$$

$$+ \frac{1}{4\pi^2} \iint\limits_{\mathbb{R}^2 \setminus [-t^{-\frac{1}{\alpha}}\pi, t^{-\frac{1}{\alpha}}\pi]^2} e^{-h(v,w)} dv\, dw, \tag{6.3.12}$$

where χ_G is the characteristic function of a set $G \subseteq \mathbb{R}^2$. The integral in (6.3.12) converges to 0 as $t \to \infty$; note that the integral in (6.3.12) exists by (6.3.10). From (6.3.9) and (6.3.10) we obtain the following estimate for the integrand in (6.3.11):

$$\begin{aligned}
&\chi_{[-t^{-\frac{1}{\alpha}}\pi, t^{-\frac{1}{\alpha}}\pi]^2}(v,w) \Big| e^{-tl(t^{-\frac{1}{\alpha}}v, t^{-\frac{1}{\alpha}}w)} - e^{-h(v,w)} \Big| \\
&\leq \chi_{[-t^{-\frac{1}{\alpha}}\pi, t^{-\frac{1}{\alpha}}\pi]^2}(v,w) \Big(e^{-tl(t^{-\frac{1}{\alpha}}v, t^{-\frac{1}{\alpha}}w)} + e^{-h(v,w)} \Big) \\
&\leq \chi_{[-t^{-\frac{1}{\alpha}}\pi, t^{-\frac{1}{\alpha}}\pi]^2}(v,w) \Big(e^{-tC(t^{-1}|v|^\alpha + t^{-1}|w|^\alpha)} + e^{-C_1(|v|^\alpha + |w|^\alpha)} \Big) \\
&\leq e^{-C(|v|^\alpha + |w|^\alpha)} + e^{-C_1(|v|^\alpha + |w|^\alpha)},
\end{aligned}$$

where the right-hand side is integrable on $\mathbb{R}^2$ and independent of t. For fixed $v, w \in \mathbb{R}^2$ and large enough $t > 0$ we have

$$\begin{aligned}
tl\big(t^{-\frac{1}{\alpha}}v, t^{-\frac{1}{\alpha}}w\big) &= th\big(t^{-\frac{1}{\alpha}}v, t^{-\frac{1}{\alpha}}w\big) + tR\big(t^{-\frac{1}{\alpha}}v, t^{-\frac{1}{\alpha}}w\big) \\
&= h(v,w) + t\, o\big(t^{-1}\big(|v|^\alpha + |w|^\alpha\big) \to h(v,w) \qquad \text{as } \ t \to \infty.
\end{aligned}$$

Hence the integrand in (6.3.11) converges to 0 pointwise as $t \to \infty$. Now the Dominated Convergence Theorem implies that the integral in (6.3.11) converges to 0 as $t \to \infty$. Since the integrals in (6.3.11) and (6.3.12) are independent of ξ and η, the convergence in (6.3.7) is uniform in ξ and η.

The relation in (6.3.8) follows easily from (6.3.7) by using the substitution $x = t^{\frac{1}{\alpha}}\xi$, $y = t^{\frac{1}{\alpha}}\eta$. □

The next theorem is the main result of this chapter. It contains the long-time

behaviour of the solution of the Cauchy problem corresponding to the Mellin-transformed k-path Laplacian. It shows, in particular, that for $s \in (2,4)$ the solution exhibits superdiffusive behaviour whereas for $s > 4$ one has normal diffusion.

Theorem 6.10. *Let $\Gamma = (V,E)$ be the square lattice as described at the beginning of Section 6.2, let $s > 2$, $s \neq 4$, and let $l_{M,s}$ be the Mellin-transformed k-path Laplacian defined in* (6.2.10)*. Let u be the solution in* (6.2.20) *of* (6.2.16), (6.2.17) *with $\mathring{u} = e_{0,0}$, where $e_{0,0}$ is defined in* (6.2.19)*. Then*

$$u_{x,y}(t) = t^{-\frac{2}{\alpha}} F_s\big(t^{-\frac{1}{\alpha}}x, t^{-\frac{1}{\alpha}}y\big) + o\big(t^{-\frac{2}{\alpha}}\big), \qquad t \to \infty, \tag{6.3.13}$$

uniformly in $x, y \in \mathbb{Z}$, where in the case $s \in (2,4)$,

$$\alpha = s-2 \qquad \text{and} \qquad F_s(\xi,\eta) := \frac{1}{4\pi^2} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i(\xi v+\eta w)} e^{-h_{1,s}(v,w)}\, dv\, dw,$$

with $h_{1,s}$ from Proposition 6.8, and in the case $s \in (4,\infty)$,

$$\alpha = 2 \qquad \text{and} \qquad F_s(\xi,\eta) := \frac{1}{4\pi\gamma_s} e^{-\frac{\xi^2+\eta^2}{4\gamma_s}},$$

with

$$\gamma_s = \frac{\zeta(s-1) + 2\zeta(s-3)}{3}\,.$$

(See Figs. 6.3.2 and 6.3.3).

Proof. By Proposition 6.8 and Lemma 6.2 the function $l_{M,s}$ satisfies the assumptions of Lemma 6.9 with $h = h_{1,s}$ and $\alpha = s-2$ when $s \in (2,4)$ and with $h = h_{2,s}$ and $\alpha = 2$ when $s \in (4,\infty)$. Hence all claims follow from Lemma 6.9. □

Remark 6.11. Theorem 6.10 shows that the distribution spreads proportionally to $t^{\frac{1}{\alpha}}$ where α is as in that theorem; cf. Remark 5.6. When $s > 4$, one has

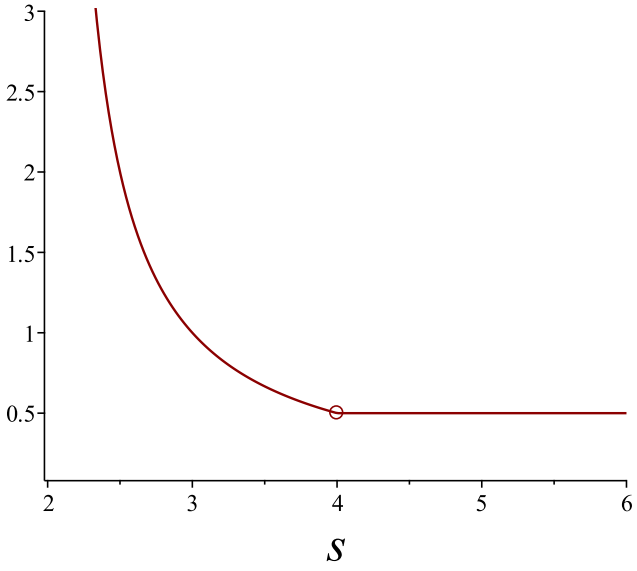
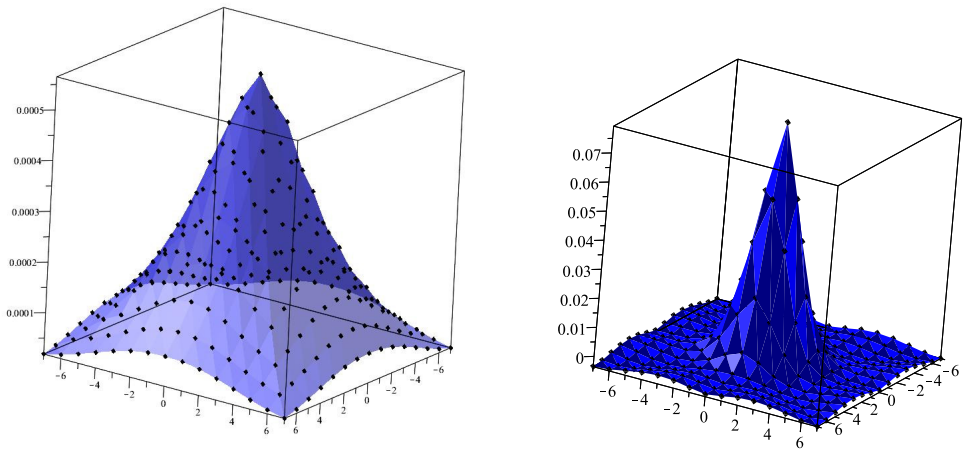


Figure 6.3.2: The s-dependance of $\frac{1}{\alpha}$.



(a) $s = 2.5$ (b) $s = 6$

Figure 6.3.3: The graph of the limit solution F_s from Theorem 6.10 for $s = 2.5$ (a) and $s = 6$ (b), respectively. The black dots indicate the result of numerical integration of (6.2.20), whereas the blue curve indicate the asymptote (6.3.13).

normal diffusion since the profile spreads proportionally to $t^{\frac{1}{2}}$ in this case. When $2 < s < 4$, however, we observe superdiffusion because then the spread of the profile is proportional to t^{κ} with $\kappa = \frac{1}{s-2} > \frac{1}{2}$. In particular, when $s = 3$, then the profile spreads linearly in time, which is a ballistic behaviour.

One can measure the spread, e.g. with the full width at half maximum (FWHM), which, for our purpose, we can define as (6.9)

$$FWHM(t) := 2\sup\Big\{r > 0 : u_{x,y}(t) \le \frac{1}{2}u_{0,0}(t) \quad \text{for all } x, y \in \mathbb{Z} \text{ with } |x|^2 + |y|^2 \ge r^2\Big\}.$$

One can show that $FWHM(t) \sim ct^{\frac{1}{\alpha}}$ as $t \to \infty$ with some $c > 0$; cf. Remark 5.6 for the one-dimensional case.

Remark 6.12. Let us consider finite truncations of the Mellin transformation (6.2.10) of the k-path Laplacian, i.e. set

$$L_{M,s,N} := \sum_{k=1}^{N} \frac{1}{k^s} L_k,$$

for $N \in \mathbb{N}$. By Lemma 6.1 this operator is unitarily equivalent to the operator of multiplication by the function

$$l_{M,s,N}(p,q) = \sum_{k=1}^{N} \frac{1}{k^s} l_k(p,q),$$

where l_k is defined in that lemma. Using Lemmas 6.4 and 6.5 one can show in a similar way as above that

$$l_k(p,q) = \frac{2k^3 + k}{3}(p^2 + q^2) + O(p^4 + q^4), \qquad p, q \to 0,$$

and hence

$$l_{M,s,N} = \sum_{k=1}^{N} \frac{2k^3 + k}{3k^s}(p^2 + q^2) + O(p^4 + q^4), \qquad p, q \to 0.$$

Although this leads to normal distribution by Lemma 6.9, the variance of the limiting normal distribution grows with N. If one measures this with the full width at half maximum one gets

$$FWHM(t) \sim 2\left((\ln 2)\sum_{k=1}^{N} \frac{2k^3 + k}{3k^s}\right)^{\frac{1}{2}} t^{\frac{1}{2}}, \qquad t \to \infty; \tag{6.3.14}$$

cf. Remark 5.8. As $N \to \infty$ one has the following behaviour,

$$\sum_{k=1}^{N} \frac{(2k^2+1)k}{3k^s} \sim \frac{2}{3(4-s)} N^{4-s}, \qquad N \to \infty, \qquad \text{if } s \in (2,4),$$

$$\sum_{k=1}^{N} \frac{(2k^2+1)k}{3k^s} \to \frac{2\zeta(s-3) + \zeta(s-1)}{3}, \qquad N \to \infty, \qquad \text{if } s \in (4,\infty).$$

Note that when $s > 4$, the limiting distributions converge to the limiting distribution from Theorem 6.10. When $2 < s < 4$, the coefficient in (6.3.14) diverges as $N \to \infty$.

6.4 Summary

In this chapter the results for the superdiffusive behaviour of a solution are applied to the *Abstract Cauchy Problem* corresponding to transformed k-path LOs on 2-dimensional graphs. This work focusses on the Cartesian grid particularly square lattice. Theorem 6.10 describes the asymptotic behaviour of the generalised diffusion equation corresponding to the Mellin-transformed k-path Laplacian and encapsulates the main result of the current chapter. Superdiffusion is proven to occur when $2 < s < 4$ and that normal diffusion is the rule when $s > 4$. More

particularly, the time evolution of the solution of the generalised diffusion equation with the initial condition concentrated at one point is investigated. As time t tends to infinity, the spread of the solution (e.g. measured by the full width at half maximum) grows, similar to t^k, where $k = 1/2$ when $s > 4$, which is normal diffusion, and where $k > 1/2$ when $2 < s < 4$, which is superdiffusive behaviour.

Chapter 7

Conclusions and Future Works

7.1 Conclusions

The generalised k-path LOs and their transforms, namely the, Laplace, Factorial and Mellin for connected and locally finite infinite graphs have been introduced. This generalisation is based on the k-path LOs, which account for the hop of a diffusive particle to its non-nearest neighbours in a graph. The probability that the particle jumps to its non-nearest neighbours declines with the distance separating the target from the original position. A discrete model was constructed, in which control points characterising the space are situated in the nodes of a network and the distances between them are calculated as the shortest path between vertices. First, it has been conclusively shown that the k-path LOs are well-defined, closed and self-adjoined operators. Subsequently, it has been proved that the operator k-path LOs, defined on the infinite networks, are bounded if and only if the k-path degree of vertices is bounded. It has furthermore been proven that all three transformed k-path LOs under certain conditions are self-adjoint and bounded. Furthermore, we studied the diffusion on an infinite graph, obtaining analytical expressions for the transformed k-path LOs as well as for the exponential operators of both the k-path Laplacians and their transformations. Here

we have introduced a new theoretical framework to describe superdiffusion by a transformation of k-path LOs defined on certain graphs. In this case, $1D$ and $2D$ infinite graphs have been employed. First, we numerically study the transformed k-path Laplacians for a linear chain with numerous nodes. We have analytically revealed that the density profile asymptotically converges to stable distributions. When the Laplace and factorial transformed operators are used in a generalised diffusion equation, the diffusive processes observed are always normal independent of the transform parameters. The asymptotic profile is always Gaussian. For the Mellin transformed k-path Laplacians, the diffusion is normal only when the exponent s in the transform $c_k = k^{-s}$ is greater than, or equal to, three. For values of $1 < s < 3$, the signature of superdiffusive processes was observed. The asymptotic profile is not Gaussian - rather a Levy-type stable distribution. It has been revealed that the anomalous diffusion observed for these values of the Mellin transform is produced by the probabilities of big jumps of the Mellin transformed Laplacian operators, which differs to a large extent from those of the Laplace and factorial transformations. Second, a natural extension of the above-mentioned theory to the existence of anomalous diffusion on a square lattice was reviewed, whereby we defined the Mellin transformed k-path LOs on a square lattice, showing that a Mellin's transformed k-path LO is well-defined, bounded, self-adjoint and non-negative. This allows us to describe a process where the diffusive particle can jump any number of edges with a probability that depends on the length of the jump. A superdiffusive behaviour on a square lattice corresponding to Mellin transforms of the k-path Laplacian was noted. We have proved that the superdiffusion process can be obtained for a Mellin's transformed k-path LO in the Cartesian grid with the parameter s in the interval (2, 4).

7.2 Future Works

The results in this thesis establish a solid mathematical foundation for network analysis. Through this research, some ideas have evolved that could be listed as directions for future research:

- Extending the current results to the study of a generalised Schrödinger equation using the transformed k-path Laplacian operators in similar lines to those we have employed.
- Extending the current results to an infinite hexagonal lattice (grid) as well as other infinite networks with particular kinds of structures.
- Studying the generalised diffusion equation with the different transforms for real-world networks.

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