PATH LAPLACIAN OPERATORS AND SUPERDIFFUSIVE PROCESSES ON GRAPHS. I. ONE-DIMENSIONAL CASE

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Abstract. We consider a generalization of the diffusion equation on graphs. This generalized diffusion equation gives rise to both normal and superdiffusive processes on infinite one-dimensional graphs. The generalization is based on the k-path Laplacian operators L_k, which account for the hop of a diffusive particle to non-nearest neighbours in a graph. We first prove that the k-path Laplacian operators are self-adjoint. Then, we study the transformed k-path Laplacian operators using Laplace, factorial and Mellin transforms. We prove that the generalized diffusion equation using the Laplace- and factorial-transformed operators always produce normal diffusive processes independently of the parameters of the transforms. More importantly, the generalized diffusion equation using the Mellin-transformed k-path Laplacians $\sum_{k=1}^{\infty} k^{-s} L_k$ produces superdiffusive processes when $1 < s < 3$.

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1. Introduction

Superdiffusive processes are ubiquitous in many natural systems, ranging from physical to biological and man-made ones. They refer to those anomalous diffusive processes where the mean square displacement (MSD) of the diffusive particle scales nonlinearly with time. We refer the reader to [20] and the references therein for the background and applications of anomalous diffusion. The superdiffusive processes have been modelled in many different ways (see [20] for a review and analysis). The most used models, however, are based on random walks with Lévy flights (RWLF) [7] and on the use of the fractional diffusion equation (FDE) [2, Chapter 11]. There are different types of definitions of fractional derivative, such as the Caputo fractional operator and the Riemann–Liouville fractional operator [25], which then have different interpretations and adapt differently to the different physical phenomena studied with them (see [10, 17]).

Recently, anomalous diffusion of ultracold atoms has been observed in a discrete one-dimensional system [27]. The model considered in that work for explaining the superdiffusive process is 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. Then, after some time the particles' position is distributed in a non-Gaussian way and the full width at half maximum (FWHM) scales as a power-law of the time with a signature characteristic of superdiffusion. The mathematical framework used to describe this anomalous diffusion was based on the FDE. However, an alternative view of this process is possible. First, we can consider that the diffusive particle is diffusing in a one-dimensional discrete space. Then, we can consider that the diffusive particle is not only hopping to its nearest neighbours in the 1D lattice, but to any other point of it with a probability that scales with the distance between the two places. In the current work we prove analytically that such kind of processes can give rise to superdiffusion under certain conditions. We

should remark that existence of such long-range hops in diffusive process has been well documented since the 1990s on experimental basis of different nature. First, the group of G. Ehrlich [28] 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 adatom and admolecules diffusing on metallic surfaces has been confirmed in many different systems [33, 1].

The study of diffusion on graphs is a well-established physico-mathematical theory based on the graph-theoretic version of the diffusion equation [15, 16]

$$\frac{\mathrm{d}}{\mathrm{d}t}u(t) = -Lu(t), \tag{1.1}$$

$$u(0) = u_0, \tag{1.2}$$

where L — the discrete Laplacian — is defined via the adjacency matrix A of the graph and the diagonal matrix of vertex degrees K as $L = K - A$ [22, 19, 21]. The Laplacian matrix has been extended to infinite, connected and locally finite graphs and studied as an operator in the Hilbert space ℓ^2 over the vertices [3, 29, 11, 14, 12, 31, 32, 9]. Although RWLF and the FDE have been applied to study diffusion on graphs (see for instance [30, 18]), the question that arises here is whether is it possible to design a simple graph-theoretic, physically sound and mathematically elegant method based on a generalization of the Laplacian operator in (1.1) to account for the superdiffusive process observed in physical phenomena. An appropriate scenario for this generalization is to consider that the diffusive particle can hop not only to its nearest neighbours — as controlled by L in (1.1) — but to any other node of the graph, with a probability that decays with the increase of the shortest path distance separating the node in which the particle is currently located to the one to which it will hop. A generalization of the Laplacian matrix — known as the k-path Laplacian — that takes into account such long-range hops of the diffusive particle has been recently considered for finite undirected graphs [8].

The aim of this article is twofold. First, we extend the k-path Laplacians L_k [8] to consider connected and locally finite infinite graphs. We prove here that these operators are self-adjoint. We also study the transformed k-path Laplacian operators using Laplace, factorial and Mellin transforms. We then study an infinite linear chain and obtain analytical expressions for the transformed k-path Laplacians operators as well as for the exponential operators of both, the k-path Laplacians and their transformations. Second, we plug this generalized Laplacian operators into the graph-theoretic diffusion equation (1.1–1.2) to obtain a generalized diffusion equation for graphs. We prove that when the Laplace- and factorial-transformed operators are used in the generalized diffusion equation, the diffusive processes observed are always normal independently of the parameters of the transforms. For the Mellin-transformed k-path Laplacians $\sum_{k=1}^{\infty} k^{-s} L_k$ we find that the diffusion is normal only when $s > 3$. 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 $(1, \infty)$. We remind that in general we can find that MSD $\sim t^{\kappa}$, where the diffusion is *normal* when $\kappa = 1$, while it is a superdiffusive process when $\kappa > 1$. The particular case when $\kappa = 2$ is known as *ballistic* diffusion, which is characterized by the fact that at small times the particles are not hindered yet by collisions and diffuse very fast. In a follow-up paper (Part II) we shall study the two-dimensional situation.

2. The k-path Laplacian operators

In this work we always consider $\Gamma = (V, E)$ to be an undirected finite or infinite graph with vertices V and edges E. We assume that Γ is connected and locally finite (i.e. each vertex has only finitely many edges emanating from it). Let d be the distance metric on Γ, 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.

$$\delta_k(v) := \#\{w \in V : d(v, w) = k\}. \tag{2.1}$$

Since Γ 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

$$\langle f, g\rangle = \sum_{v\in V} f(v)\overline{g(v)}, \qquad f, g \in \ell^2(V). \tag{2.2}$$

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

$$e_v(w) := \begin{cases} 1 & \text{if } w = v, \\ 0 & \text{otherwise.} \end{cases} \tag{2.3}$$

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

$$\big(\mathcal{L}_k f\big)(v) := \sum_{w\in V:\, d(v,w)=k} \big(f(v) - f(w)\big), \qquad f \in C(V). \tag{2.4}$$

This means that by replacing L in (1.1) by $\mathcal{L}_k$ in (2.4) we obtain a diffusive process in which the diffusive particle hops to nodes which are separated by k edges from its current location. This represents a natural extension of the idea of diffusion on graphs where the particle can only hops to nearest neighbours from its current position. As it has been analysed in [8], the so-called k-path Laplacian naturally extends the concept of graph connectivity, i.e. whether a graph is connected or not, to the k-connectivity, which indicates whether every node in the graph can be reached by a particle which is k-hopping from node to node in the graph.

On the vectors e_v it acts as follows:

$$(\mathcal{L}_k e_v)(w) = \begin{cases} \delta_k(v) & \text{if } w = v, \\ -1 & \text{if } d(v, w) = k, \\ 0 & \text{otherwise.} \end{cases} \tag{2.5}$$

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

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

respectively. Clearly, $e_v \in \operatorname{dom}(L_{k,\min})$, and we obtain from (2.5) that

$$\big\|L_{k,\min} e_v\big\| = \sqrt{\big(\delta_k(v)\big)^2 + \delta_k(v)} = \begin{cases} 0 & \text{if } \delta_k(v) = 0, \\ \delta_k(v)\sqrt{1 + \dfrac{1}{\delta_k(v)}} & \text{if } \delta_k(v) > 0. \end{cases} \tag{2.6}$$

First we show that $L^*_{k,\min} = L_{k,\max}$. To this end let $f \in C_0(V)$ and $g \in C(V)$, let V_{00} be the support of f and set

$$V_0 := V_{00} \cup \big\{v \in V : \exists\, w \in V_{00} \text{ such that } d(v, w) = k\big\}, \tag{2.7}$$

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

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

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

$$= \frac{1}{2}\sum_{\substack{v,w\in V_0:\\ d(v,w)=k}} \big(f(v)-f(w)\big)\overline{\big(g(v)-g(w)\big)} \tag{2.8}$$

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

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

$$= \sum_{v\in V} f(v)\overline{(\mathcal{L}_k g)(v)}. \tag{2.9}$$

Let $g \in \operatorname{dom}(L_{k,\max})$. It follows from (2.9) that

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

for all $f \in \operatorname{dom}(L_{k,\min})$, which implies that $g \in \operatorname{dom}(L^*_{k,\min})$. Now let $g \in \operatorname{dom}(L^*_{k,\min})$. For each $v \in V$ we obtain from (2.9) 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 $g \in \operatorname{dom}(L_{k,\max})$. 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 (2.8) that

$$\big\langle L_{k,\min} f, f\big\rangle = \frac{1}{2}\sum_{\substack{v,w\in V_0:\\ d(v,w)=k}} \big|f(v)-f(w)\big|^2, \tag{2.10}$$

where V_0 is as in (2.7); this shows that $L_{k,\min}$ is a non-negative operator.

We say that a subset V_0 of V is *k-connected* if each pair $v, w \in V_0$ is connected by a k-hopping walk. The set $V_0 \subset V$ is called a *k-connected component* of V if V_0 is a maximal k-hopping connected subset of V. If $V_0 \subset V$ is a k-hopping component, then $C(V_0)$ considered as a subspace of $C(V)$ is $\mathcal{L}_k$-invariant.

Lemma 2.1. *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*

$$\big(\mathcal{L}_k f\big)(v) \le 0 \quad \textit{for every } v \in V_0, \tag{2.11}$$

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 (2.11). Hence f is constant on V_0. □

Next we show that $L_{k,\min}$ is actually essentially self-adjoint; see, e.g. [11, 31, 32] for the case $k = 1$.

Theorem 2.2. *The operator $L_{k,\min}$ is essentially self-adjoint and hence $L_{k,\max}$ is equal to the closure of $L_{k,\min}$.*

Proof. Since $L_{k,\min}$ is non-negative and $L_{k,\min}^* = L_{k,\max}$, it is sufficient 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

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

Now we consider the function $|f|$:

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

Since $f|_{V_0} \in \ell^2(V_0)$, the function $|f|$ attains the supremum on V_0. Hence Lemma 2.1 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 forms: for $f \in \mathrm{dom}(L_{k,\min}) = C_0(V)$ we obtain from (2.10) that

$$\begin{aligned}\big\langle L_{k,\min} f, f\big\rangle &= \frac{1}{2} \sum_{\substack{v,w\in V:\\ d(v,w)=k}} \big|f(v)-f(w)\big|^2 \le \frac{1}{2} \sum_{\substack{v,w\in V:\\ d(v,w)=k}} \Big(|f(v)|+|f(w)|\Big)^2 \\ &\le \sum_{\substack{v,w\in V:\\ d(v,w)=k}} \Big(|f(v)|^2+|f(w)|^2\Big) \\ &= \sum_{v\in V} \delta_k(v)|f(v)|^2 + \sum_{w\in V} \delta_k(w)|f(w)|^2 \\ &= 2\sum_{v\in V} \delta_k(v)|f(v)|^2. \end{aligned} \tag{2.12}$$

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

Theorem 2.3. *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*

$$\delta_{k,\max} := \max\{\delta_k(v) : v \in V\}; \tag{2.13}$$

then

$$\delta_{k,\max} \le \|L_k\| \le 2\delta_{k,\max}. \tag{2.14}$$

Proof. If δ_k is unbounded, then (2.6) immediately shows that L_k is unbounded. Now assume that δ_k is bounded. Relation (2.6) yields the lower bound for $\|L_k\|$ in (2.14). From (2.12) we obtain that for $f \in \mathrm{dom}(L_{k,\min})$,

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

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 $\|L_k\| \le 2\delta_{k,\max}$. □

3. Transformed k-path Laplacian operators

We consider series of the form

$$\sum_{k=1}^{\infty} c_k L_k \tag{3.1}$$

with $c_k \in \mathbb{C}$. If all L_k are bounded and

$$\sum_{k=1}^{\infty} |c_k|\,\|L_k\| < \infty, \tag{3.2}$$

then the series in (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 (3.1) is self-adjoint; if $c_k \ge 0$ for all $k \in \mathbb{N}$, then it is a non-negative operator.

In the following we discuss three transformed operators in more detail: the Laplace, the factorial and the Mellin transforms.

Theorem 3.1. *Assume that δ_1 is bounded on V and let $\delta_{1,\max}$ be as in* (2.13).

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

$$\widetilde{L}_{\mathrm{L},\lambda} := \sum_{k=1}^{\infty} e^{-\lambda k} L_k \tag{3.3}$$

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

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

$$\widetilde{L}_{\mathrm{F},z} := \sum_{k=1}^{\infty} \frac{z^k}{k!} L_k \tag{3.4}$$

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*

$$\delta_{k,\max} \leq Ck^{\alpha} \tag{3.5}$$

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

$$\widetilde{L}_{\mathrm{M},s} := \sum_{k=1}^{\infty} \frac{1}{k^s} L_k \tag{3.6}$$

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

Under the assumption (3.5) *the operator* $\widetilde{L}_{\mathrm{L},\lambda}$ *from* (3.3) *is bounded for every* $\lambda \in \mathbb{C}$ *with* $\operatorname{Re} \lambda > 0$.

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 2.3. Therefore the convergence condition (3.2) is satisfied in items (i) and (ii) for the specified λ and z.

For item (iii) we observe that under the condition (3.5) the operators L_k satisfy

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

Hence also in this case the condition (3.2) is satisfied for $\widetilde{L}_{\mathrm{M},s}$ with $\operatorname{Re} s > \alpha + 1$ and for $\widetilde{L}_{\mathrm{L},\lambda}$ with $\operatorname{Re} \lambda > 0$. □

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 (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. 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 [13, §VI.1.5] 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

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

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

$$\sum_{k=1}^{N} c_k \mathfrak{l}_k \tag{3.7}$$

is an increasing sequence of densely defined, closed, non-negative quadratic forms (see [13, Theorem VI.1.31]). By [13, Theorem VIII.3.13a] the sequence in (3.7) converges to a closed non-negative quadratic form $\tilde{\mathfrak{l}}$ that is given by

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

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

Assume now that

$$\sum_{k=1}^{\infty} c_k \delta_k(v) < \infty \tag{3.8}$$

for every $v \in V$. Since

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

by (2.5), condition (3.8) implies that $e_v \in \operatorname{dom}(\tilde{\mathfrak{l}})$ for every $v \in V$, and hence the form $\tilde{\mathfrak{l}}$ is densely defined. By [13, Theorem VI.2.1] there exists a self-adjoint non-negative operator $\tilde{L}$ that corresponds to $\tilde{\mathfrak{l}}$ in the sense that

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

Moreover, [13, 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

$$\delta_k(v) \le (n+k)!$$

for each vertex v in generation n. For $z \in (0,1)$ condition (3.8) is satisfied for the factorial transform since

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

for every vertex v in generation n. Hence $\widetilde{L}_{\mathrm{F},z}$ 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 $c_k \ge 0$ and that condition (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 $\tilde{\mathfrak{l}}[Cf] \le \tilde{\mathfrak{l}}[f]$ for every mapping $C : \mathbb{C} \to \mathbb{C}$ with $C(0) = 0$ and $|Cx - Cy| \le |x - y|$. By the Beurling–Deny criteria the operator $-\tilde{L}$ generates an analytic, positivity-preserving semigroup of contractions; see, e.g. [26, Appendix 1 to Section XIII.12]. In the remaining sections we consider a situation where all L_k are bounded operators and (3.2) is satisfied. In this case we can write $(e^{-t\tilde{L}})_{t \ge 0}$ for the semigroup.

4. The k-path Laplacians on the infinite path graph

Let P_∞ be the infinite path graph (or chain), 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

$$(L_k)_{\mu\nu} = 2\delta_{\mu,\nu} - \delta_{\mu,\nu-k} - \delta_{\mu,\nu+k}, \qquad \mu,\nu \in \mathbb{Z}, \tag{4.1}$$

where δ denotes the Kronecker delta.

In order to consider the diffusion of particles on the graph, we let e_0 be as in (2.3), i.e.

$$(e_0)_n = \delta_{n,0}, \tag{4.2}$$

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 $\widetilde{L}_{\mathrm{L},\lambda}$, $\widetilde{L}_{\mathrm{F},z}$ and $\widetilde{L}_{\mathrm{M},s}$ from (3.3), (3.4) and (3.6), respectively, are bounded operators for $\lambda \in \mathbb{C}$ with $\operatorname{Re}\lambda > 0$, for every $z \in \mathbb{C}$ and every $s \in \mathbb{C}$ with $\operatorname{Re} s > 1$. 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 4.1. *Let $\lambda \in \mathbb{C}$ with $\operatorname{Re}\lambda > 0$, $z \in \mathbb{C}$ and $s \in \mathbb{C}$ with $\operatorname{Re} s > 1$, and let $\widetilde{L}_{\mathrm{L},\lambda}$, $\widetilde{L}_{\mathrm{F},z}$, $\widetilde{L}_{\mathrm{M},s}$ be as in (3.3), (3.4) and (3.6), respectively. Then for any $u \in \ell^2(P_\infty)$ we have*

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

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

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

where ζ is Riemann's zeta function defined by

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

Applying them to e_0 we obtain

$$\big(\widetilde{L}_{\mathrm{L},\lambda}e_0\big)_n = \begin{cases} \dfrac{2}{e^\lambda - 1} & \text{if } n = 0, \\ e^{-\lambda|n|} & \text{if } n \neq 0, \end{cases} \qquad \big(\widetilde{L}_{\mathrm{F},z}e_0\big)_n = \begin{cases} 2(e^z - 1) & \text{if } n = 0, \\ \dfrac{z^{|n|}}{|n|!} & \text{if } n \neq 0, \end{cases} \tag{4.3}$$

$$\big(\widetilde{L}_{\mathrm{M},s}e_0\big)_n = \begin{cases} 2\zeta(s) & \text{if } n = 0, \\ \dfrac{1}{|n|^s} & \text{if } n \neq 0. \end{cases} \tag{4.4}$$

Proof. Let c_k, $k \in \mathbb{N}$, be arbitrary coefficients so that (3.2) 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 follow easily. □

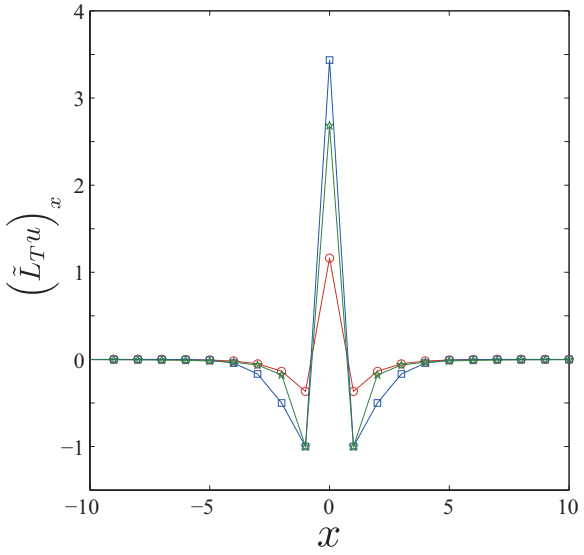

FIGURE 4.1. Plot of the particle density at the different nodes of a linear path with 21 nodes obtained from the Laplace (circles), factorial (squares) and Mellin (stars) transformed k-path Laplacians with $\lambda = 1$, $z = 1$ and $s = 2.5$, respectively.

Figure 4.1 illustrates the results of Lemma 4.1 in a graphical form displaying $\widetilde{L}_{\mathrm{L},1}e_0$, $\widetilde{L}_{\mathrm{F},1}e_0$ and $\widetilde{L}_{\mathrm{M},2.5}e_0$ 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. Time-evolution operators

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

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

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

$$u(t) = e^{-tL}w, \qquad t \geq 0. \tag{5.1}$$

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

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

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

$$\ell_k(q) := 2 - e^{ikq} - e^{-ikq} = 2\big(1 - \cos(kq)\big), \tag{5.2}$$

i.e.

$$\big(\mathcal{F}L_k\mathcal{F}^{-1}g\big)(q) = \ell_k(q)g(q), \qquad g \in L^2(-\pi,\pi). \tag{5.3}$$

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

$$\big(\mathcal{F}\widetilde{L}_T\mathcal{F}^{-1}g\big)(q) = \tilde{\ell}_T(q)g(q) \tag{5.4}$$

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

$$\begin{gathered}\tilde{\ell}_{\mathrm{L},\lambda}(q) := \sum_{k=1}^{\infty} e^{-\lambda k}\ell_k(q), \qquad \tilde{\ell}_{\mathrm{F},z}(q) := \sum_{k=1}^{\infty} \frac{z^k}{k!}\ell_k(q), \\ \tilde{\ell}_{\mathrm{M},s}(q) := \sum_{k=1}^{\infty} \frac{1}{k^s}\ell_k(q).\end{gathered} \tag{5.5}$$

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

Lemma 5.1. *Let $\lambda \in \mathbb{C}$ with $\operatorname{Re}\lambda > 0$, $z \in \mathbb{C}$, $s \in \mathbb{C}$ with $\operatorname{Re} s > 1$. With the notation from above we have*

$$\tilde{\ell}_{\mathrm{L},\lambda}(q) = \frac{(e^\lambda + 1)(1 - \cos q)}{(e^\lambda - 1)(\cosh\lambda - \cos q)}\,, \tag{5.6}$$

$$\tilde{\ell}_{\mathrm{F},z}(q) = 2\big[e^z - e^{z\cos q}\cos(z\sin q)\big], \tag{5.7}$$

$$\tilde{\ell}_{\mathrm{M},s}(q) = 2\zeta(s) - \mathrm{Li}_s(e^{iq}) - \mathrm{Li}_s(e^{-iq}), \tag{5.8}$$

where Li_s is the polylogarithm — also known as Jonquière's function — defined for $s \in \mathbb{C}$ with $\operatorname{Re} s > 1$ by

$$\mathrm{Li}_s(z) := \sum_{k=1}^{\infty} \frac{z^k}{k^s} \qquad \text{when } |z| \le 1$$

and by analytic continuation to $\mathbb{C} \setminus (1,\infty)$.

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

$$\ell(q) > 0 \qquad \text{for } q \in [-\pi,\pi] \setminus \{0\} \tag{5.9}$$

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

Proof. Representation (5.6) follows from

$$\begin{aligned}\tilde{\ell}_{\mathrm{L},\lambda}(q) &= 2\sum_{k=1}^{\infty} e^{-\lambda k} - \sum_{k=1}^{\infty} e^{-\lambda k}e^{ikq} - \sum_{k=1}^{\infty} e^{-\lambda k}e^{-ikq} \\ &= \frac{2}{e^{\lambda}-1} - \frac{1}{e^{\lambda-iq}-1} - \frac{1}{e^{\lambda+iq}-1} = \frac{2}{e^{\lambda}-1} - 2\frac{e^{\lambda}\cos q - 1}{\left|e^{\lambda-iq}-1\right|^2} \\ &= \frac{2}{e^{\lambda}-1} - 2\frac{e^{\lambda}\cos q - 1}{e^{2\lambda}+1-2e^{\lambda}\cos q} = \frac{2}{e^{\lambda}-1} - \frac{\cos q - e^{-\lambda}}{\cosh\lambda - \cos q} \\ &= \frac{(e^{\lambda}+1)(1-\cos q)}{(e^{\lambda}-1)(\cosh\lambda-\cos q)}\,.\end{aligned}$$

The representations (5.7) and (5.8) are proved easily. The continuity of the functions follows from the representations (5.6)–(5.8) or from the uniform convergence of the series.

To show (5.9), 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 (5.5) 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; cf., e.g. [4, Proposition 2] for a similar representation for the case $L = L_1$.

Theorem 5.2. *Let $\lambda \in \mathbb{C}$ with $\operatorname{Re}\lambda > 0$, $z \in \mathbb{C}$ and $s \in \mathbb{C}$ with $\operatorname{Re} s > 1$, let $L = L_k$, $\widetilde{L}_{\mathrm{L},\lambda}$, $\widetilde{L}_{\mathrm{F},z}$ or $\widetilde{L}_{\mathrm{M},s}$ and let $\ell = \ell_k$, $\tilde{\ell}_{\mathrm{L},\lambda}$, $\tilde{\ell}_{\mathrm{F},z}$ or $\tilde{\ell}_{\mathrm{M},s}$, correspondingly. For $w = (w_\nu)_{\nu\in\mathbb{Z}} \in \ell^2(P_\infty)$ the solution of (5.1) is given by*

$$\big(u(t)\big)_n = \big(e^{-tL}w\big)_n = \sum_{\nu\in\mathbb{Z}} w_\nu \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(n-\nu)q}e^{-t\ell(q)}\,\mathrm{d}q, \qquad t \geq 0,\ n \in \mathbb{Z}. \quad (5.10)$$

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

$$\big(e^{-tL}\big)_{\mu\nu} = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i(\mu-\nu)q}e^{-t\ell(q)}\,\mathrm{d}q = \frac{1}{2\pi}\int_{-\pi}^{\pi} \cos\big((\mu-\nu)q\big)e^{-t\ell(q)}\,\mathrm{d}q. \quad (5.11)$$

Proof. Since $\mathcal{F}L\mathcal{F}^{-1}$ acts as a multiplication operator by ℓ (see (5.3) and (5.4)), we have

$$\big(\mathcal{F}e^{-tL}\mathcal{F}^{-1}g\big)(q) = e^{-t\ell(q)}g(q), \qquad g \in L^2(-\pi,\pi).$$

Let $\nu \in \mathbb{Z}$ and e_ν as in (2.3). Then

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

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 (5.10) and hence also (5.11). □

In Figure 5.1 we illustrate the time evolution of the density $u(t)$ for the three transforms of the k-path Laplace operators.

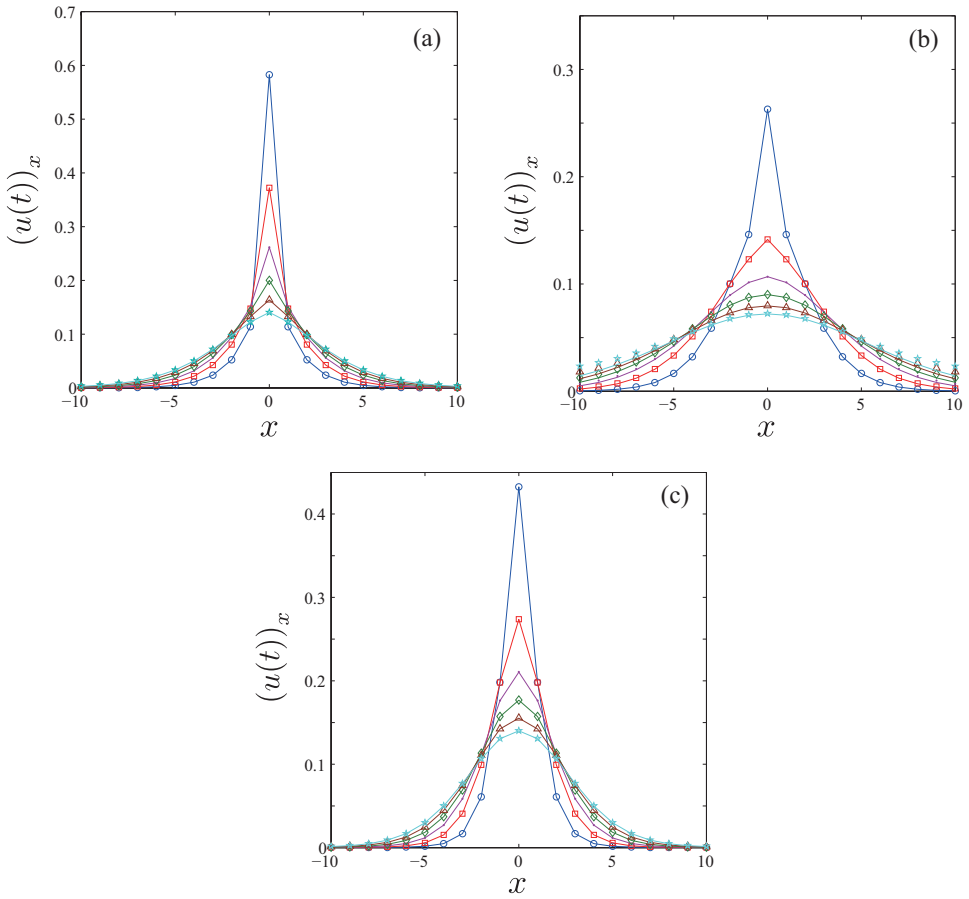

FIGURE 5.1. The particle density $(u(t))_x$ as a function of x for the transformed k-path Laplacians for a linear chain with 21 nodes. The symbols indicate the results obtained from the simulations of the linear chain and the solid lines represent the values obtained analytically from Theorem 5.2 for 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 $s = 4$.

6. Generalized diffusion on the path graph

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

$$\frac{\mathrm{d}}{\mathrm{d}t}u(t) = -Lu(t), \tag{6.1}$$

$$u(0) = e_0, \tag{6.2}$$

where e_0 is as in (4.2) and L is any of the transformed k-path Laplacians $\widetilde{L}_{\mathrm{L},\lambda}$, $\widetilde{L}_{\mathrm{F},z}$ or $\widetilde{L}_{\mathrm{M},s}$, approaches a stable distribution if appropriately scaled. Stable distributions can be parameterized with four parameters as follows (see, e.g. [23, §1.3]). Let $\alpha \in (0, 2]$, $\beta \in [-1, 1]$, $\gamma > 0$ and $\delta \in \mathbb{R}$; then the density of the stable distribution $S(\alpha, \beta, \gamma, \delta)$ is given by

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

where

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

with

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

Note that $\phi(\,\cdot\,;\alpha,\beta,\gamma,\delta)$ is the characteristic function of the probability distribution $S(\alpha,\beta,\gamma,\delta)$. We are only interested in the case when $\beta = \delta = 0$, which yields the following simpler function:

$$\phi(z;\alpha,0,\gamma,0) = \exp\big(-|\gamma z|^\alpha\big). \tag{6.3}$$

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:

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

When $\alpha < 2$ the density has a power-like decay:

$$f(\xi;\alpha,0,\gamma,0) \sim \frac{1}{\pi}\Gamma(\alpha+1)\sin\Big(\frac{\pi\alpha}{2}\Big)\gamma^\alpha\cdot\frac{1}{\xi^{\alpha+1}} \qquad \text{as } \xi \to \pm\infty; \tag{6.4}$$

see, e.g. [23, Theorem 1.12]. 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 $x \to 0$. Relation (6.4) implies that $S(\alpha,0,\gamma,0)$ has no finite variance if $\alpha < 2$. Further, if $\alpha \le 1$, then even the first moment is infinite.

In the following we study the asymptotic behaviour of the density profile $u(t)$ that solves (6.1) and (6.2). It follows from (5.10) that

$$\big(u(t)\big)_x = \big(e^{-tL}e_0\big)_x = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ixq}e^{-t\ell(q)}\,\mathrm{d}q, \qquad x \in \mathbb{Z},\ t \ge 0. \tag{6.5}$$

In the next lemma we consider the asymptotic behaviour of integrals as in (6.5). We allow also values $\alpha > 2$ in the notation $f(z;\alpha,0,\gamma,0)$ although this is not needed later.

Lemma 6.1. *Let $\alpha > 0$ and let $h : [-\pi,\pi] \to \mathbb{R}$ be a continuous function that satisfies*

$$h(q) > 0 \qquad \text{for } q \in [-\pi,\pi]\setminus\{0\}, \tag{6.6}$$

$$h(q) \sim c|q|^\alpha \qquad \text{as } q \to 0 \tag{6.7}$$

with some $c > 0$. Then

$$t^{\frac{1}{\alpha}}\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{it^{\frac{1}{\alpha}}\xi q}e^{-th(q)}\,\mathrm{d}q \to \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\xi z}e^{-c|z|^\alpha}\,\mathrm{d}z \tag{6.8}$$

$$= f\big(\xi;\alpha,0,c^{\frac{1}{\alpha}},0\big) \tag{6.9}$$

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

Hence

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ixq}e^{-th(q)}\,\mathrm{d}q = t^{-\frac{1}{\alpha}} f\big(t^{-\frac{1}{\alpha}}x;\alpha,0,c^{\frac{1}{\alpha}},0\big) + \mathrm{o}\big(t^{-\frac{1}{\alpha}}\big) \tag{6.10}$$

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

$$\begin{aligned}
&\left| t^{\frac{1}{\alpha}}\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{it^{\frac{1}{\alpha}}\xi q}e^{-th(q)}\,\mathrm{d}q - \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\xi z}e^{-c|z|^\alpha}\,\mathrm{d}z\right| \\
&= \left|\frac{1}{2\pi}\int_{-\pi t^{\frac{1}{\alpha}}}^{\pi t^{\frac{1}{\alpha}}} e^{i\xi z}e^{-th(t^{-\frac{1}{\alpha}}z)}\,\mathrm{d}z - \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\xi z}e^{-c|z|^\alpha}\,\mathrm{d}z\right| \\
&\le \left|\frac{1}{2\pi}\int_{-\pi t^{\frac{1}{\alpha}}}^{\pi t^{\frac{1}{\alpha}}} e^{i\xi z}\Big(e^{-th(t^{-\frac{1}{\alpha}}z)} - e^{-c|z|^\alpha}\Big)\,\mathrm{d}z\right| \\
&\quad + \left|\frac{1}{2\pi}\int_{\mathbb{R}\setminus[-\pi t^{\frac{1}{\alpha}},\pi t^{\frac{1}{\alpha}}]} e^{i\xi z}e^{-c|z|^\alpha}\,\mathrm{d}z\right| \\
&\le \frac{1}{2\pi}\int_{-\pi t^{\frac{1}{\alpha}}}^{\pi t^{\frac{1}{\alpha}}} \left|e^{-th(t^{-\frac{1}{\alpha}}z)} - e^{-c|z|^\alpha}\right|\mathrm{d}z \qquad (6.11) \\
&\quad + \frac{1}{2\pi}\int_{\mathbb{R}\setminus[-\pi t^{\frac{1}{\alpha}},\pi t^{\frac{1}{\alpha}}]} e^{-c|z|^\alpha}\,\mathrm{d}z. \qquad (6.12)
\end{aligned}$$

First note that the integrals in (6.11) and (6.12) are independent of ξ. We show that both integrals converge to 0 as $t \to \infty$. For the integral in (6.12) this is clear. Let us now consider the integral in (6.11). Since h is continuous and satisfies (6.6) and (6.7), the function $q \mapsto h(q)/|q|^\alpha$ is bounded below by a positive constant, i.e. there exists $\tilde{c} > 0$ such that

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

This implies that the integrand in (6.11) 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 (6.11) 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 (6.7) 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 (6.11) converges to 0 as $t \to \infty$. This shows (6.8).

Finally, we prove (6.10). With the substitution $x = t^{\frac{1}{\alpha}}\xi$ we obtain from (6.8) and (6.9) that

$$\frac{1}{t^{-\frac{1}{\alpha}}}\left|\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ixq}e^{-th(q)}\,\mathrm{d}q - t^{-\frac{1}{\alpha}} f\big(t^{-\frac{1}{\alpha}}x;\alpha,0,c^{\frac{1}{\alpha}},0\big)\right|$$

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

uniformly in $x \in \mathbb{R}$ as $t \to \infty$, which shows (6.10). □

Remark 6.2. The lemma can be interpreted as follows. If the function

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

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

$$\big(u(t)\big)_0 \sim t^{-\frac{1}{\alpha}} f\big(0;\alpha,0,c^{\frac{1}{\alpha}},0\big) = \frac{\Gamma\big(\frac{\alpha+1}{\alpha}\big)}{\pi c^{\frac{1}{\alpha}}} t^{-\frac{1}{\alpha}}, \qquad \text{as } t \to \infty. \tag{6.13}$$

The full width at half maximum (FWHM) increases like

$$\mathrm{FWHM}(t) \sim 2\xi_0 t^{\frac{1}{\alpha}} \qquad \text{as } t \to \infty, \tag{6.14}$$

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 $(\mathrm{FWHM}(t))^2 \sim ct^{\kappa}$ 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 $\alpha < 2$. ◊

6.1. **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. [6] for the case $L = L_1$). This is caused by the fact that ℓ_k, $\tilde{\ell}_{\mathrm{L},\lambda}$ and $\tilde{\ell}_{\mathrm{F},z}$ behave quadratically around 0.

Theorem 6.3. *Let P_∞ be the infinite path graph, let $\lambda, z > 0$ and let $\widetilde{L}_{\mathrm{L},\lambda}$ and $\widetilde{L}_{\mathrm{F},z}$ be the Laplace-transformed and factorial-transformed k-path Laplacian with parameters λ and z, respectively. Moreover, let $u(t)$ be the solution of* (6.1), (6.2) *with $L = L_k$, $L = \widetilde{L}_{\mathrm{L},\lambda}$ or $L = \widetilde{L}_{\mathrm{F},z}$. Then*

$$\big(u(t)\big)_x = t^{-\frac{1}{2}} \frac{1}{2\sqrt{\pi a}} \exp\left(-\frac{x^2}{4at}\right) + \mathrm{o}\big(t^{-\frac{1}{2}}\big) \qquad \textit{as } t \to \infty \tag{6.15}$$

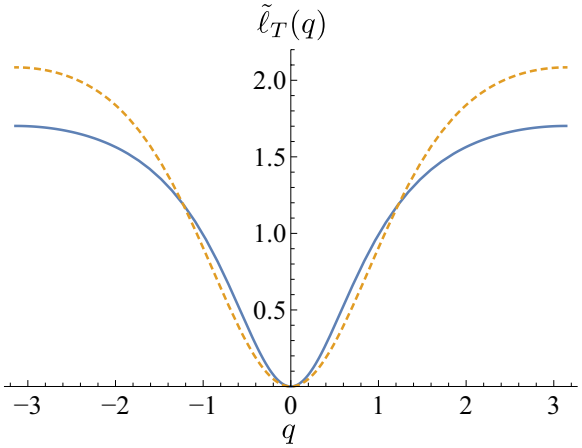

FIGURE 6.1. The graphs of the functions $\tilde{\ell}_{\mathrm{L},\lambda}$ with $\lambda = 1$ (blue solid curve) and $\tilde{\ell}_{\mathrm{F},z}$ with $z = 1/2$ (orange broken curve) on the interval $[-\pi, \pi]$.

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

$$a = k^2 \qquad \text{for } L = L_k, \tag{6.16}$$

$$a = \frac{e^\lambda \left(e^\lambda + 1\right)}{(e^\lambda - 1)^3} = \frac{\coth\left(\frac{\lambda}{2}\right)}{2(\cosh\lambda - 1)} \qquad \text{for } L = \widetilde{L}_{\mathrm{L},\lambda}, \tag{6.17}$$

$$a = z(z+1)e^z \qquad \text{for } L = \widetilde{L}_{\mathrm{F},z}. \tag{6.18}$$

Proof. The asymptotic behaviour of the functions ℓ_k, $\tilde{\ell}_{\mathrm{L},\lambda}$ and $\tilde{\ell}_{\mathrm{F},z}$ from (5.2), (5.6) and (5.7) is $\ell_k(q) \sim k^2 q^2$ as $q \to 0$,

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

with a from (6.17) and

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

with a from (6.18), respectively. Now (6.15) follows from (6.5) and Lemma 6.1. □

Remark 6.4. Theorem 6.3 shows that the diffusion for the k-path Laplacian, the Laplace-transformed and the factorial-transformed k-path Laplacian is always 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 (6.16)–(6.18); see (6.13). 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

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

see (6.14). For the limiting behaviour after rescaling in x see Remark 6.2. ◊

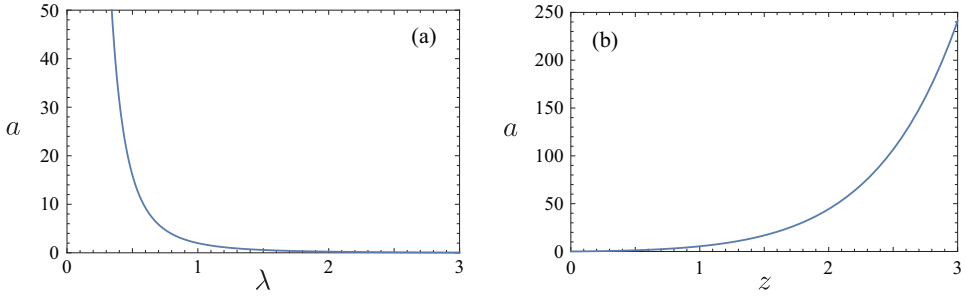

FIGURE 6.2. The parameter dependence of a for (a) the Laplace-transformed and (b) the factorial-transformed k-path Laplacian.

6.2. **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 $s > 3$.

Theorem 6.5. *Let P_∞ be the infinite path graph, let $s > 1$ and let $\widetilde{L}_{\mathrm{M},s}$ be the Mellin-transformed k-path Laplacian with parameter s. Moreover, let $u(t)$ be the solution of (6.1) and (6.2) with $L = \widetilde{L}_{\mathrm{M},s}$. Then*

$$\big(u(t)\big)_x = t^{-\frac{1}{\alpha}} f\big(t^{-\frac{1}{\alpha}}x;\alpha,0,\gamma,0\big) + \mathrm{o}\big(t^{-\frac{1}{\alpha}}\big) \qquad \text{as } t\to\infty \tag{6.19}$$

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

$$\alpha = s-1, \quad \gamma = \left(-\frac{\pi}{\Gamma(s)\cos\big(\frac{\pi s}{2}\big)}\right)^{\frac{1}{s-1}} \qquad \text{if } 1<s<3, \tag{6.20}$$

$$\alpha = 2, \qquad \gamma = \sqrt{\zeta(s-2)} \qquad \text{if } s>3. \tag{6.21}$$

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

$$f(\xi;\alpha,0,\gamma,0) \sim \frac{1}{\xi^s} \qquad \text{as } \xi\to\pm\infty, \tag{6.22}$$

where α and γ are as in (6.20).

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

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

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

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

Proof. We consider the behaviour of $\tilde{\ell}_{\mathrm{M},s}$ from (5.8) at 0. Let $s > 1$ with $s \notin \mathbb{N}$. It follows from [24, 25.12.12] that

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

which yields

$$\begin{aligned}\tilde{\ell}_{\mathrm{M},s}(q) &= 2\zeta(s) - \mathrm{Li}_s(e^{iq}) - \mathrm{Li}_s(e^{-iq})\\ &= 2\zeta(s) - \Gamma(1-s)\Big((-iq)^{s-1} + (iq)^{s-1}\Big) - \sum_{n=0}^{\infty}\zeta(s-n)\frac{(iq)^n + (-iq)^n}{n!}\end{aligned}$$

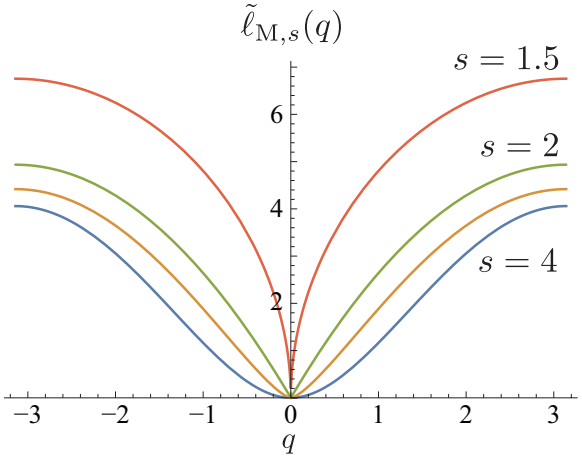

FIGURE 6.3. The graphs of the functions $\tilde{\ell}_{\mathrm{M},s}$ on the interval $[-\pi, \pi]$. The parameter s is varied from top to the bottom as 1.5, 2, 2.5 (not labelled) and 4.

$$= -\Gamma(1-s)|q|^{s-1}\left(e^{-i(s-1)\frac{\pi}{2}} + e^{i(s-1)\frac{\pi}{2}}\right) - \sum_{n=1}^{\infty} \zeta(s-n)\frac{(iq)^n + (-iq)^n}{n!}$$

$$= -\frac{\pi}{\Gamma(s)\sin(\pi s)}|q|^{s-1} 2\cos\left(\frac{(s-1)\pi}{2}\right) - \sum_{l=1}^{\infty} \zeta(s-2l)\frac{2(-1)^l q^{2l}}{(2l)!}$$

$$= -\frac{\pi}{\Gamma(s)\cos\left(\frac{s\pi}{2}\right)}|q|^{s-1} - \sum_{l=1}^{\infty} \zeta(s-2l)\frac{2(-1)^l q^{2l}}{(2l)!} \tag{6.23}$$

$$= -\frac{\pi}{\Gamma(s)\cos\left(\frac{s\pi}{2}\right)}|q|^{s-1} + \zeta(s-2)q^2 + \mathrm{O}(q^4) \tag{6.24}$$

as $q \to 0$. By continuity (6.23) and hence (6.24) are also valid for $s = 2$. If $s < 3$, then the first term in (6.24) is dominating; if $s > 3$, then the second term is dominating. Hence

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

as $q \to 0$. Now (6.19) follows from (6.5) and Lemma 6.1.

To show (6.22), we use (6.4), 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 $\tilde{\ell}_{\mathrm{M},s}(q)$ involves a logarithmic term, which implies that the asymptotic behaviour of $(u(t))_x$ is more complicated.

Remark 6.6. In Fig. 6.4 we plot the density profiles for various times when the time evolution is governed by (6.1) with L being the Mellin-transformed k-path

Laplacian $\widetilde{L}_{\mathrm{M},s}$. The peak height is attained at $x = 0$ and behaves like

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

as $t \to \infty$, where γ is as in (6.20); see (6.13). If $s \in (1,3)$, then the full width at half maximum (FWHM) behaves like

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

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 (6.14). 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 6.2. ◊

Remark 6.7. Consider the operator

$$L = cL_1^a \tag{6.25}$$

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 6.1 that

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

when u is a solution of (6.1), (6.2) with L as in (6.25). 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 6.5. However, the solutions behave differently for small t as can be seen from Figure 6.6 where the blue solid line with circles corresponds to $L = \widetilde{L}_{\mathrm{M},s}$ and the red dashed line with squares corresponds to $L = cL_1^a$ for $t = 1$ (a) and $t = 3$ (b). See [5] for a discussion of L_1^a where it was also shown that (6.1), (6.2) with $L = L_1^a$ is equivalent to an evolution equation with a fractional time derivative ([5, Theorem 3]). ◊

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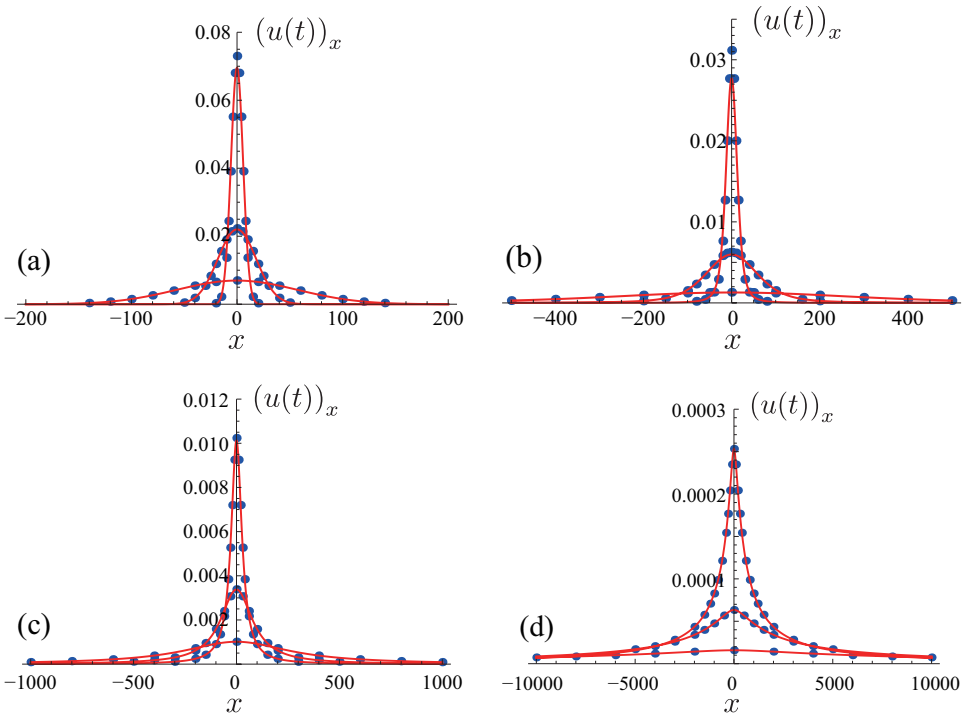

FIGURE 6.4. The time evolution of the density profile under the Mellin-transformed k-path Laplacian: (a) $s = 4$ for $t = 10, 100, 1000$ from high to low; (b) $s = 2.5$ for $t = 10, 100, 1000$ from high to low; (c) $s = 2$ for $t = 10, 30, 100$ from high to low; (d) $s = 1.5$ for $t = 10, 20, 40$ from high to low. In every panel, the blue dots indicate the result of numerical integration of (6.5) with $\ell = \tilde{\ell}_{\mathrm{M},s}$, whereas the red curves indicate the asymptote (6.19).

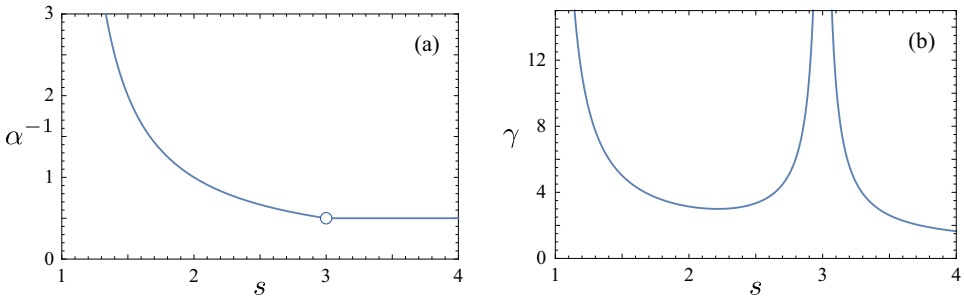

FIGURE 6.5. The s-dependence of (a) $1/\alpha$ and (b) γ.

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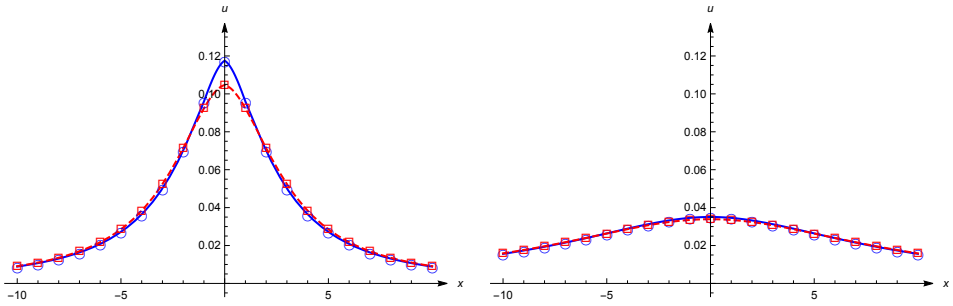

(a) (b)

FIGURE 6.6. The solutions of (6.1), (6.2) for $L = \widetilde{L}_{\mathrm{M},s}$ (blue solid line with circles) and for $L = cL_1^a$ (red dashed line with squares) for $t = 1$ (a) and $t = 3$ (b).

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