d-PATH LAPLACIAN OPERATORS ON NETWORKS. FROM CLASSICAL TO QUANTUM DIFFUSION

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Introduction

Recently I have defined the d-path Laplace operators L_d [1] in a similar way as the standard graph Laplacian, but taking into account those pairs of nodes whose topological distance is equal to d. Hence L_d describes hops to nodes at distance d from its origin. We have then studied transformations of L_d as combinations of the form $\sum_{d=1}^{\Delta} c_d L_d$ with some non-negative coefficients c_d, and where $\varDelta$ is the graph diameter. We have proved that when $c_d = d^{-s}$, with some positive parameter s, a generalized diffision equation on infinite 1- [2] and 2-dimensional graphs [3] produces superdiffusive behaviors. The choice of the transformation has proved to be crucial in determining the diffusive behaviour because it appears when a Mellin transform of the d-path Laplace operators is considered with s satisfying $1 < s < 3$ (1D) or $2 < s < 4$ (2D), but normal diffusion is observed either $s > 3$ (1D) or $s > 4$ (2D) or when one considers different transformations of L_d like the Laplace and factorial transforms.

Preliminaries

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 shortest path distance metric on Γ, i.e. $d(v, w)$ is the length of the shortest path from v to w, and let $\delta_d(v)$ be the d-path degree of the vertex v [1, 2], i.e.

$$\delta_d(v) = \#\{w \in V : d(v, w) = d\}. \tag{0.1}$$

Let $\ell^2(V)$ be the Hilbert space of square-summable functions on V with inner product

$$\langle f, g\rangle = \sum_{v \in V} f(v)\overline{g(v)}, \qquad f, g \in \ell^2(V). \tag{0.2}$$

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

$$e_v(w) = \begin{cases} 1 & \text{if } w = v, \\ 0 & \text{otherwise.} \end{cases} \tag{0.3}$$

For $d \in \mathbb{N}$ the following operator defined in $\ell^2(V)$ is the d-path Laplacian of the graph

$$\big(L_d f\big)(v) := \sum_{w \in V:\, d(v,w)=d} \big(f(v) - f(w)\big), \tag{0.4}$$

$f \in \operatorname{dom}(L_d)$ which act on the vectors e_v it acts as follows:

$$(L_d e_v)(w) = \begin{cases} \delta_d(v) & \text{if } w = v, \\ -1 & \text{if } d(v, w) = k, \\ 0 & \text{otherwise.} \end{cases} \tag{0.5}$$

For each $d \in \mathbb{N}$ the d-path Laplacian L_d is a self-adjoined operator in $\ell^2(V)$. Furthermore, the operator L_d is bounded if and only if the function $\delta_d : V \to \mathbb{N}$ is bounded.
Let $\mathscr{L}_s$ be the *Mellin-transformed d-Laplacian*

$$\mathscr{L}_s := \sum_{d=1}^{\triangle} d^{-s} L_d, \tag{0.6}$$

where $s \in \mathbb{R}^+$.

Main results

Here I will consider the study of quantum transport with long-range hops on graphs. For that I will plug the transformed d-path Laplacian operators into the Schrödinger equation without potential to obtain

$$\frac{\partial \vec{\Psi}(t)}{\partial t} = -i\mathscr{L}_s \vec{\Psi}(t), \vec{\Psi}(0) = \vec{\Psi}_0, \quad (0.7)$$

where $\mathscr{L}_s$ is the Mellin transformed d-path Laplacians as defined before. The solution of the Schrödinger equation with the transformed d-path Laplacian operators is $\exp(-\vec{it}\mathscr{L}_s)\Psi_0$, where

$$\exp(-it\mathscr{L}_s) = U\exp(-it\Lambda)U^{-1}. \quad (0.8)$$

For the analysis of quantum transport on graph it is common to consider the *transition probability* between two nodes p and q, $\pi_{pq}(s,t)$, at a given time t and for a given values of the parameter s,

$$\pi_{pq}(s,t) = \left| \sum_{j=1}^{n} e^{-it\mu_j(\mathscr{L}_s)} \psi_{j,p}\psi_{j,q} \right|^2. \quad (0.9)$$

In particular, $\pi_{pp}(s,t)$ is the return probability to the node p and $\bar{\pi}(s,t) = \frac{1}{n}\sum_{p=1}^{n} \pi_{pp}(s,t)$ is the *average probability of return*. We are going to analyze the evolution of the quantum transport in some simple graphs.

Then, I will find analytical expressions for the transition and return probabilities of a quantum particle at the nodes of a ring graph. I will show that the average return probability in ring graphs decays as a power law with time when long-range interactions (LRI) are present.

In contrast, I prove analytically that the transition and return probabilities on a complete and start graphs oscillate around a constant value. This allowed to infer that in a barbell graph–a graph consisting of two cliques separated by a path–the quantum particle get trapped and oscillates across the nodes of the path without visiting the nodes of the cliques. I then compare the use of the Mellin-transformed d-path Laplacian operators versus the use of fractional powers of the combinatorial Laplacian [4] to account for LRI. Apart from some important differences observed at the limit of the strongest LRI, the d-path Laplacian operators produces the emergence of new phenomena related to the location of the wave packet in graphs with barriers, which are not observed neither for the Schrödinger equation without LRI nor for the one using fractional powers of the Laplacian.

References

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