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EDGE-BASED LINEAR WAVE EQUATIONS ON QUANTUM TREES WITH DIRICHLET VERTEX CONDITIONS AND ITS SIMULATION

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Abstract. We investigate the linear wave equations on the quantum trees S_N and $P_2 \rhd S_2$ with Dirichlet vertex conditions at each leaf vertex. We first determine the edge-based Laplacian spectra on the quantum tree using quantitative analysis of the scattering matrix. This yields edge-based Laplacian spectral properties in the quantum trees S_N and $P_2 \rhd S_2$, which we use to determine the general solution of the linear wave equation. Furthermore, we provide a solution to the wave equation with a Gaussian wave packet as an initial condition. We present an example of our numerical simulation.

Досліджуються лінійні хвильові рівняння на квантових деревах S_N і $P_2 \rhd S_2$ з вузловими умовами Діріхле на кожній вершині ребра. Спочатку визначаємо спектр лапласіана для кожного вузла на квантовому дереві за якісного аналізу матриці розсіювання. Це дає спектральні властивості лапласіана на кожному ребрі для квантових дерев S_N і $P_2 \rhd S_2$, який далі використовується для визначення загального розв'язку лінійного хвильового рівняння. Крім того, розв'язано хвильове рівняння з хвильовим пакетом Гауса в якості початковій умови. Наведемо приклад чисельного моделювання.

1. Introduction

A linear wave equation on graphs has been discussed extensively since early 2000. Friedman and Tillich in [7] use edge-based Laplacian to model a linear wave equation on a graph and determine a solution based on the Laplacian eigensystem. In 2019, Aziz [2] explored the linear wave model and determined the solution to classify the structure of graphs or networks. This graph classification method was started by Aziz in [1], and further explored by Gajewski in [8]. Both Friedmann and Aziz used adjacency calculus to determine the Laplacian spectrum. Furthermore, the vertex conditions given to the vertices are only Neumann-Kirchhoff type. The graph is assumed to be equilateral, that is, the graph has edges of a uniform length or weight. A comprehensive discussion of Laplacian eigensystem can be found in Wilson's work [12] published in 2013.

Many types of quantum graphs can be used for a precision physical model in biology problems, such as the wave equation in trees as a model for blood flow, see Carlson 2006 [6]. A Quantum tree has a particular structure with leaf vertices (that is, the vertices with degree one) to which we can assign the Dirichlet vertex condition. In graph-theoretic terminology, a tree is a graph that does not contain cycles. In this paper, we solve the linear wave equation on an equilateral quantum tree with the Dirichlet vertex condition at the leaf vertices. The two types of trees used in this paper are the star graph S_N and the tree $P_2 \rhd S_2$. The star graph S_N is a special type of graphs in which N vertices have degree 1 and a single vertex has degree N. This looks like the N vertices are connected to a single common interior vertex. A star graph with total of $N+1$-vertices is denoted by S_N. The tree $P_2 \rhd S_2$ combines three trees: two star graphs S_2 and one graph P_2, where P_2 is simply an interval, that is a graph consisting of two vertices connected by one edge. In contrast to Aziz's work in 2019 and our previous results [5], here we determine the

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edge-based Laplacian spectrum using the scattering matrices as in [3, 4, 9]. This spectral analysis approach has some advantages, including obtaining edge-based Laplacian spectra for quantum graphs with Dirichlet vertex conditions and non-equilateral graphs.

Our main result in this direction is obtaining some properties of the scattering matrix and the edge-based Laplacian spectrum on the S_N and $P_2 \triangleright S_2$ along with their eigenfunctions. Furthermore, we obtain a solution of the edge-based linear wave equation on equilateral quantum trees with Dirichlet vertex conditions at each of its leaf vertices. These results include formulas distinct from that of Aziz et al. 2019 [2]. Our method works for arbitrary (connected) graphs.

This article is arranged in the following order. In Section 2, we mentioned and focus on the concept of metric trees, Laplacian, vertex conditions at vertices, a system of eigenvalue problems, and secular determinants using scattering matrices. Section 3 contains our main results. The first result deals with properties of the scattering matrix in the star graph S_N, followed by the Laplacian spectrum of S_N and $P_2 \triangleright S_2$ along with their eigenfunctions. The second result is the general solution for the edge-based wave equation on S_N and $P_2 \triangleright S_2$, with the Gaussian wave packet initial data. In Section 4, we present a simulation of wave evolution on the star graphs S_3, S_4, and $P_2 \triangleright S_2$ with Gaussian wave packet as initial data.

2. Preliminaries

In this section, we provide some basic notions and terminologies so that we can bring some machinery used in differential equations into graphs under consideration. Our primary references for this purpose are [3, 4, 7, 9].

Let $T = (V, E)$ be a directed tree with the set of vertices V and the set of directed edges E, which we assume to be nonempty and finite. Next, we assume that the tree T is nonempty, directed, connected, finite, and simple (see [4, 9]). Each directed edge e can be identified with a pair of vertices $(o(e), t(e))$; that is, $o(e)$ and $t(e)$ are the origin vertex and the terminal vertex, respectively. The edge $e = (o(e), t(e))$ is parameterized by the interval $[0, L_e]$, with relation $0 \longleftrightarrow o(e)$ and $L_e \longleftrightarrow t(e)$, where L_e is any positive real number which, by physical consideration, can be considered as length or weight of the edge e. We let E_v to be the set of all edge incidences to the vertex v, that is,

$$E_v = \{e \in E : v = o(e) \text{ or } v = t(e)\}.$$

The degree d_v of the vertex v is the cardinality of E_v. The boundary set ∂T of a tree T is the set of all vertex having degree one. An element of the boundary set is called a leaf vertex, denoted by v_{leaf}. Meanwhile $v_{int} \in V \backslash \partial T$ is called an interior vertex of the tree T.

Let $\mathcal{I}_T = \cup_{e\in E}(\{e\} \times (0, L_e))$. The *metric tree* $\tilde{T}$ based on T is the set

$$\tilde{T} = \mathcal{I}_T \cup V.$$

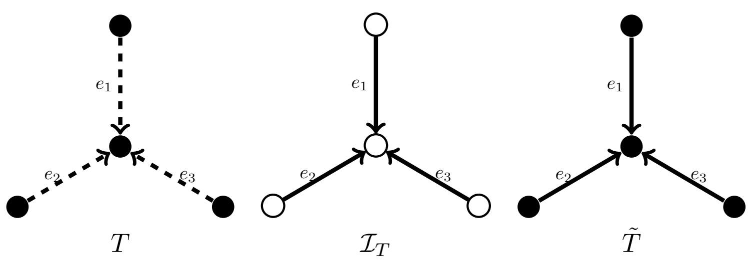

Figure 1. Illustrates T, $\mathcal{I}_T$, and $\tilde{T}$ for a simple star tree S_3.

The set $\mathcal{I}_T$ can be considered as interior of the metric tree $\tilde{T}$. For alternative definitions of metric trees (metric graphs), see [4, 11]. Furthermore, a metric tree is called equilateral if all L_e are identically 1. Next, we denote T_m as the pair $\left(\tilde{T}, m\right)$, where $\tilde{T}$ is the metric tree and m is the metric on $\tilde{T}$. Based on the Lebesgue measure on each interval $[0, L_e]$, a Lebesgue measure on the metric tree T_m can be defined [7].

There is a one to one correspondence between functions f on T_m and families $\{f_e : e \in E\}$ of functions f_e defined on intervals $[0, L_e]$ which satisfy the following compatibility condition:

$$f_{e_i}(v_{int}) = f_{e_j}(v_{int}),$$

where v_{int} is identified with the corresponding end-point of the interval $[0, L_{e_i}]$, resp., $[0, L_{e_j}]$.

Linear differential operators on graphs have been discussed in [4, 10, 7]. In this paper, we use edge-based Laplacian notions introduced by Friedman and Tillich in 2004. The edge-based Laplacian is negative Laplacian, that is, the negative second derivative. The Laplacian acting on the function $f = (f_e)$ is

$$\triangle_T f = \frac{d^2 f_e}{dx_e^2}, \qquad e \in E.$$

The domain of the Laplacian is defined as

$$D(\triangle_T) := \{f = (f_e) : f_e \in H^2([0, L_e]) : f_e \text{ satisfy the vertex conditions}, e \in E\},$$

where H^2 denotes the Sobolev space of functions on the interval $[0, L_e]$ whose second derivative is square integrable. The Sobolev space on the metric tree is $\widetilde{H}^2(T_m) := \oplus_{e\in E} H^2([0, L_e])$ with the norm

$$\|f\|^2_{\widetilde{H}^2(T_m)} := \sum_{e\in E} \|f_e\|^2_{H^2([0,L_e])}, \qquad f \in \widetilde{H}^2(T_m) \text{ and } f = (f_e),\ e \in E.$$

Recall that the norm

$$\|f_e\|^2_{H^2([0,L_e])} := \|f_e\|^2_{L^2([0,L_e])} + \|f_e'\|^2_{L^2([0,L_e])} + \|f_e''\|^2_{L^2([0,L_e])} \text{ for every } f_e \in H^2([0, L_e]).$$

A quantum tree is a metric tree T_m equipped with a differential operator $\mathcal{H}$, accompanied by conditions at the vertices (vertex condition). Next, we write the quantum tree as an ordered pair $(T_m, \mathcal{H})$. There are two types of vertex conditions on a vertex in what follows, which will be used in the next section.

Let $|V|$ and $|E|$ are the cardinalities of the sets V and E, respectively. We define the signed incidence matrix $(q_{v,e})_{|V|\times|E|}$ by

$$q_{v,e} = \begin{cases} -1, & \text{if } v = o(e), \\ 1, & \text{if } v = t(e), \\ 0, & \text{others.} \end{cases}$$

The Neumann-Kirchoff vertex condition at a vertex $v_{int} \in V \backslash \partial T$ is

$$\sum_{e\in E_{v_{int}}} q_{v_{int},e} f_e'(v_{int}) = 0,$$

and the Dirichlet vertex condition at a vertex $v_{leaf} \in \partial T$ is $f_e(v_{leaf}) = 0$.

Next, we consider an equilateral quantum star graph S_N and an equilateral quantum tree $P_2 \rhd S_2$ with Dirichlet vertex conditions at all leaf vertices. Then the eigenvalue problem of the edge-based Laplacian on the two quantum trees is given as follows,

$$\begin{aligned} -f_e'' &= \lambda f_e && \text{for each } e \in E, \\ f_{e_i}(v_{int}) &= f_{e_j}(v_{int}) && \text{for each } e_i, e_j \in E_{v_{int}}, \\ \sum_{e \in E_{v_{int}}} q_{v_{int},e} f_e'(v_{int}) &= 0 && \text{for each } v_{int} \in V \backslash \partial T, \\ f_e(v_{leaf}) &= 0 && \text{for each } v_{leaf} \in \partial T. \end{aligned} \tag{2.1}$$

Furthermore, the two quantum trees are illustrated in Figure 2 below.

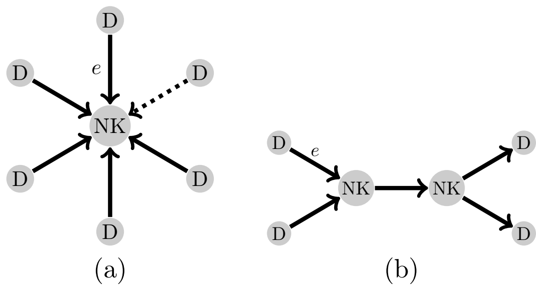

FIGURE 2. (a) Quantum star graph S_N and (b) quantum tree $P_2 \rhd S_2$. (The letters D, NK signify the Dirichlet, and Neumann-Kirchhoff vertex conditions, respectively. Where the direction of the edge e determines the parameter from 0 to 1).

2.1. **Secular Determinant.** Edge-based Laplacian spectra of a quantum graph can be calculated using its Secular Equation. This method uses the notion of a scattering matrix of a quantum graph [3, 4]. We apply the notion of secular determinants for graphs to trees.

Let $(T_m, -\Delta_T)$ be a quantum tree and $\{1, ..., |E|\}$ be the label set for its edge set. The eigenvalue problem $-\Delta_T f_j = \lambda f_j = k^2 f_j$ is given on each edge j. We express the solution on any edge j as a superposition of two plane waves,

$$f_j(x) = a_j e^{ikx} + a_{\bar{j}} e^{ik(L_j - x)}, \tag{2.2}$$

where x denotes the edge coordinate (according to the assigned direction of the edge j) and L_j the length of the edge j. The coefficient a_j is the amplitude of the plane wave moving from the coordinate $x = 0$ to $x = L_j$, and $a_{\bar{j}}$ is the amplitude of the plane wave with opposite direction. The solution is based on scattering of the plane wave e^{-ikx} coming towards the vertex v along one of the edges incident to v.

We determine the frequency k of the eigenfunctions by solving the eigenvalue problem coupled with vertex conditions at the vertices of the quantum tree. From these calculations, we obtain a matrix multiplication which describes the system of equations from the value of the plane wave amplitude on the eigenfunction,

$$SD(k)\, a = a, \tag{2.3}$$

where D is the diagonal matrix $D(k) := Diag\left(e^{ikL_j}\right)$, and the vector $a := (a_l)_{2|E| \times 1}$ with $l \in \{1, ..., |E|\} \cup \left\{\bar{1}, ..., \overline{|E|}\right\}$. The scattering matrix $S := (s_{ij}) \in \mathbb{C}^{2|E| \times 2|E|}$ is a matrix with the following entries:

$$s_{l,j} := \begin{cases} \frac{2}{d_{t(j)}} - 1, & \text{if } l = \overline{j}, \\ \frac{2}{d_{t(j)}}, & \text{if } l \neq \overline{j} \text{ and } t(j) = o(l), \\ 0, & \text{otherwise.} \end{cases}$$

Here $d_{t(j)}$ denotes the degrees of the vertex $t(j)$. The vertex condition is the Neumann-Kirchoff.

Furthermore, if we consider (2.3), we will obtain a characteristic equation that we can use to calculate the spectrum of the Laplacian.

Proposition 2.1 (Berkolaiko [3]). *Suppose $(T_m, -\Delta_T)$ is a compact quantum tree, then $k^2 \in \mathbb{C}\setminus\{0\}$ is the eigenvalue of the operator $-\Delta_T$ if only if k satisfies the equation*

$$\det(I - SD(k)) = 0,$$

where $D(k) := Diag(e^{ikL_j})$ and L_j is the length of the edge corresponding to the coefficient a_j.

The function $\Sigma(k) := \det(I - SD(k))$ is called the secular determinant. In [3, p.16,17], the relation between the representation of vertex conditions on vertices, vectors containing functions, and derivatives of functions on vertices. A local scattering matrix for vertices with Dirichlet conditions can be obtained from this relation. In the following is a scattering matrix for a quantum tree with a leaf vertex with Dirichlet conditions.

Let $(T_m, -\Delta_T)$ be a quantum tree and d_v is the degree of the vertex v. Suppose j is a directed edge with a parameterized direction corresponding to the interval $[0, L_j]$ and $\overline{j}$ is the same edge with the opposite direction. The scattering matrix S on T_m, which has the Dirichlet condition at the leaf vertices, has the following entries:

$$s_{l,j} := \begin{cases} -1, & \text{if } l = \overline{j},\ d_{t(j)} = 1, \text{ and } f(t(j)) = 0, \\ \frac{2}{d_{t(j)}} - 1, & \text{if } l = \overline{j} \text{ and } d_{t(j)} > 1, \\ \frac{2}{d_{t(j)}}, & \text{if } l \neq \overline{j} \text{ and } t(j) = o(l), \\ 0, & \text{otherwise.} \end{cases} \tag{2.4}$$

3. Results and Discussion

In this section, we discuss edge-based wave equations in quantum trees whose leaf vertices satisfy Dirichlet conditions. We begin with some facts and some properties of the scattering matrix that can be used to determine edge-based Laplacian spectra. Further, the results obtained are used to determine the solution to the edge-based wave equation.

3.1. **Some properties of the scattering matrix.**

In the following, some properties of the scattering matrix are stated. We can derive the following facts.

Lemma 3.1. *Let $(T_m, -\Delta_T)$ be an equilateral quantum tree with a scattering matrix S defined on it. Then S is a unitary matrix. If T_m is a quantum tree with all vertices (leaf and non-leaf vertices) satisfying the Neumann-Kirchoff condition, then S is row-stochastic, with eigenvalues $\alpha_1, ..., \alpha_n \in \mathbb{C}$ with $|\alpha_j| = 1$ for each $j = 1, ..., n$.*

We recall that a square matrix $S = (s_{ij}) \in \mathbb{R}^{n\times n}$ with $0 \leq s_{ij} \leq 1$ for all $1 \leq i, j \leq n$ is said to be row-stochastic if $\sum_{j=1}^{n} s_{ij} = 1$ for all $i \in \{1, ..., n\}$.

Proof. We refer to the discussion of the scattering matrix in [3, 4]. Application of the result explicitly to the eigenvalues, using the Proposition 2.1, yields the proof. □

The following theorem ensures that the scattering matrices obtained from a quantum N-star graph with different edge directions are similar. As a corollary, the eigenvalues obtained from all the scattering matrices in a quantum N-star graph are the same.

Theorem 3.2. *All the scattering matrices of the equilateral quantum star graph S_N, which have Dirichlet conditions at the leaf vertices, are similar.*

Proof. Let the standard scattering matrix $S^{(0)}$ be obtained from the parameterization $o(e_j) = v_{leaf}$ for each edge $j \in \{1, ..., N\}$, with the rows and the columns of the matrix $S^{(0)}$ being ordered according to the directed edge labels,

$$1, 2, ..., N, \quad \overline{1}, \overline{2}, ..., \overline{N}.$$

Recall that j is a directed edge with the parameterization direction corresponding to the interval $[0, L_j]$ and $\overline{j}$ is the same edge with the opposite direction.

If the equilateral quantum star graph S_N is formed by changing the parameterization of any edge, that is, there are $i \in \{1, ..., N\}$ so that $t(e_i) = v_{leaf}$, then another scattering matrix $S^{(i)}$ is obtained with the order

$$1, 2, ..., \overline{i}, ..., N, \quad \overline{1}, \overline{2}, ..., i..., \overline{N}.$$

We can choose a permutation matrix P_σ with $\sigma\left(\overline{j}\right) = j$ for $j = i$ such that

$$S^{(0)} = P_\sigma^{-1} S^{(i)} P_\sigma.$$

The statement shows that the standard scattering matrix $S^{(0)}$ is similar to every other scattering matrix of equilateral quantum star graph S_N. Thus, all scattering matrices of the equilateral quantum star graph S_N, which has the Dirichlet condition at the leaf vertices, are similar. □

Before determining the edge-based Laplacian eigensystem for trees, for convenience, we will first discuss the notion of circulant matrices.

A circulant matrix of order N, $C_N := circ(c_0, c_1, ..., c_{N-1})$, associated with the numbers $c_0, c_1, ..., c_{N-1}$ is defined as

$$C_N = \begin{pmatrix} c_0 & c_1 & \cdots & c_{N-2} & c_{N-1} \\ c_{N-1} & c_0 & \cdots & c_{N-3} & c_{N-2} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ c_2 & c_3 & \cdots & c_0 & c_1 \\ c_1 & c_2 & \cdots & c_{N-1} & c_0 \end{pmatrix},$$

where each row is a cyclic shift of the row above it. In [13], the eigenvalues of C_N are well known:

$$\lambda_j = \sum_k^{N-1} c_k \omega_j^k, \ j = 0, 1, ..., N-1,$$

where $w_j = e^{\left(\frac{2\pi i.j}{N}\right)}$ and $i = \sqrt{-1}$. Therefore, we can write the determinant of a nonsingular circulant matrix as:

$$\det(C_N) = \prod_{j=0}^{N-1} \left(\sum_k^{N-1} c_k \omega_j^k \right), \qquad k = 0, 1, ..., N-1. \tag{3.5}$$

3.2. **An edge-based Laplacian eigenvalue problem on a quantum tree which has Dirichlet conditions at all leaf vertices.** Some of the previous properties can be used to perform spectral calculations. This calculation method uses scattering matrices to obtain the Laplacian spectrum for an equilateral quantum tree, where all leaf vertices satisfy the Dirichlet condition.

Lemma 3.3 (Dirichlet spectrum). *Let $(T_m, -\Delta_T)$ be an equilateral quantum tree, with all leaf vertices satisfying the Dirichlet condition. Let S be its scattering matrix with entries as in (2.4). Suppose $\sigma(S)$ is the scattering matrix spectrum, then the Laplacian spectrum is given as follows:*

$$\sigma(-\Delta_T) = \left\{k^2 > 0 \mid e^{-ik} \in \sigma(S)\right\},$$

with the multiplicity of the eigenvalues being $m\left(k^2\right) = m\left(e^{-ik}, S\right)$.

Proof. We use secular determinants in Proposition 2.1. We have

$$\begin{aligned} 0 = |I - SD(k)| &= \left|D^{-1}(k)\, D(k) - SD(k)\right| \\ &= \left|D^{-1} - S\right| |D(k)| \\ &= \left|e^{-ik} I - S\right| |D(k)|, \end{aligned}$$

and thus e^{-ik} is the eigenvalue of the scattering matrix S. Consequently, the multiplicity of k^2 is the same as the multiplicity of e^{-ik}. □

We can see that the spectrum of the quantum tree $(T_m, -\Delta_T)$, with a Dirichlet condition at its leaf vertex, can be derived from its scattering matrix S as in the Proposition 2.1. From the lemma above, it is clear that one must first determine the eigenvalues of the S scattering matrix to obtain the Laplacian spectrum for the quantum tree.

Theorem 3.4. *Let S_N be an equilateral star graph with $N \geq 2$, with Dirichlet conditions at all leaf vertices. Suppose that $w_j = e^{\frac{2\pi i \cdot j}{N}}$. Then the characteristic polynomial for the scattering matrix of the star graph S_N is*

$$\begin{aligned} K(\alpha) &= \prod_{j=0}^{N-1} \left[\left(\alpha^2 + \left(\frac{2}{N} - 1\right)\right) + \frac{2}{N} w_j + \cdots + \left(\frac{2}{N}\right) w_j^{N-1}\right] \\ &= \left(\alpha^2 + 1\right) (\alpha - 1)^{N-1} (\alpha + 1)^{N-1}. \end{aligned}$$

Proof. Let $N \geq 2$, and S_N be an equilateral star graph, with Dirichlet conditions at all leaf vertices. According to Theorem 3.2, we can choose a standard scattering matrix of size $2N \times 2N$ which represents the star graphs, namely,

$$S = \left[\begin{array}{c|c} 0_{N\times N} & -I_{N\times N} \\ \hline P_{N\times N} & 0_{N\times N} \end{array}\right],$$

where

$$P_{N\times N} = \begin{bmatrix} \frac{2}{d_{v_{int}}} - 1 & \frac{2}{d_{v_{int}}} & \frac{2}{d_{v_{int}}} & \cdots & \frac{2}{d_{v_{int}}} \\ \frac{2}{d_{v_{int}}} & \frac{2}{d_{v_{int}}} - 1 & \frac{2}{d_{v_{int}}} & \cdots & \frac{2}{d_{v_{int}}} \\ \frac{2}{d_{v_{int}}} & \frac{2}{d_{v_{int}}} & \frac{2}{d_{v_{int}}} - 1 & \cdots & \vdots \\ \vdots & \vdots & \cdots & \ddots & \frac{2}{d_{v_{int}}} \\ \frac{2}{d_{v_{int}}} & \frac{2}{d_{v_{int}}} & \cdots & \frac{2}{d_{v_{int}}} & \frac{2}{d_{v_{int}}} - 1 \end{bmatrix}$$

and $d_{v_{int}}$ is the degree of the interior vertex. Consider the matrix $\alpha I - S$

$$\alpha I - S = \left[\begin{array}{c|c} \alpha I_{N\times N} & I_{N\times N} \\ \hline Q_{N\times N} & \alpha I_{N\times N} \end{array}\right],$$

where

$$Q_{N\times N} = \begin{bmatrix} -\left(\frac{2}{d_{v_{int}}}-1\right) & -\frac{2}{d_{v_{int}}} & -\frac{2}{d_{v_{int}}} & \cdots & -\frac{2}{d_{v_{int}}} \\ -\frac{2}{d_{v_{int}}} & -\left(\frac{2}{d_{v_{int}}}-1\right) & -\frac{2}{d_{v_{int}}} & \cdots & -\frac{2}{d_{v_{int}}} \\ -\frac{2}{d_{v_{int}}} & -\frac{2}{d_{v_{int}}} & -\left(\frac{2}{d_{v_{int}}}-1\right) & \cdots & \vdots \\ \vdots & \vdots & \cdots & \ddots & \frac{2}{d_{v_{int}}} \\ -\frac{2}{d_{v_{int}}} & -\frac{2}{d_{v_{int}}} & \cdots & -\frac{2}{d_{v_{int}}} & -\left(\frac{2}{d_{v_{int}}}-1\right) \end{bmatrix}.$$

Next, the characteristic polynomial for the scattering matrix of the star graph S_N is of the form

$$K(\alpha) = |\alpha I - S| = \left|\alpha^2 I - Q_{N\times N}\right| = 0.$$

Consider the matrix $\alpha^2 I - Q_{N\times N} = C$ as a circulant matrix of order N and, since $d_{v_{int}} = N$,

$$C = \begin{bmatrix} \alpha^2+\left(\frac{2}{N}-1\right) & \frac{2}{N} & \frac{2}{N} & \cdots & \frac{2}{N} \\ \frac{2}{N} & \alpha^2+\left(\frac{2}{N}-1\right) & \frac{2}{N} & \cdots & \frac{2}{N} \\ \frac{2}{N} & \frac{2}{N} & \alpha^2+\left(\frac{2}{N}-1\right) & \cdots & \vdots \\ \vdots & \vdots & \cdots & \ddots & \frac{2}{N} \\ \frac{2}{N} & \frac{2}{N} & \cdots & \frac{2}{N} & \alpha^2+\left(\frac{2}{N}-1\right) \end{bmatrix}$$
$$= \begin{pmatrix} c_0 & c_1 & \cdots & c_{N-2} & c_{N-1} \\ c_{N-1} & c_0 & \cdots & c_{N-3} & c_{N-2} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ c_2 & c_3 & \cdots & c_0 & c_1 \\ c_1 & c_2 & \cdots & c_{N-1} & c_0 \end{pmatrix}.$$

Let $K(\alpha) = \left|\alpha^2 I - Q_{N\times N}\right|$, then according to (3.5) we obtain

$$\begin{aligned} K(\alpha) &= \left|\alpha^2 I - Q^2_{N\times N}\right| = |C| \\ &= \prod_{j=0}^{N-1} \left(c_0 + c_1 w_j + c_2 w_j^2 + ... + c_{N-1} w_j^{N-1}\right), \end{aligned} \tag{3.6}$$

with $w_j = e^{\frac{2\pi i \cdot j}{N}}$, $c_0 = \alpha^2 + \left(\frac{2}{N}-1\right)$ and $c_1 = ... = c_{N-1} = \frac{2}{N}$.

If $j = 0$, then

$$\left(c_0 + c_1 w_j + ... + c_{N-1} w_j^{N-1}\right) = \alpha^2 + \left(\frac{2}{N}-1\right) + \frac{2}{N}(N-1),$$

so that the first factor in the product in (3.6) simplifies to

$$\left(\alpha^2+1\right).$$

Furthermore, for each $j = 1, ..., N-1$, the factors in the product in (3.6) are given by

$$(c_0 + ... + c_{N-1} w_j^{N-1}) = \alpha^2 + \left(\frac{2}{N} - 1\right) + \frac{2}{N}\left(e^{\frac{2\pi i \cdot j}{N}} + ... + \left(e^{\frac{2\pi i \cdot j}{N}}\right)^{N-1}\right).$$

Since $\sum_{n=1}^{N-1}\left(e^{\frac{2\pi i \cdot j}{N}}\right)^n = -1$, the factor is

$$\begin{aligned}(c_0 + ... + c_{N-1} w_j^{N-1}) &= \alpha^2 + \left(\frac{2}{N} - 1\right) - \frac{2}{N}\\ &= \left(\alpha^2 - 1\right).\end{aligned}$$

Therefore,

$$\begin{aligned}K(\alpha) = \left|\alpha^2 I - Q_{N\times N}\right| &= \left(\alpha^2 + 1\right)\left(\alpha^2 - 1\right)^{N-1}\\ &= \left(\alpha^2 + 1\right)(\alpha - 1)^{N-1}(\alpha + 1)^{N-1}.\end{aligned}$$

□

Next, we provide the eigenfunction formula for the eigenvalue problem (2.1) on the star graph S_N.

Corollary 3.5 (Eigenfunctions for the star graph S_N)**.** *As mentioned in Lemma 3.3, we denote eigenvalues of the scattering matrix S by α_r with $|\alpha_r| = 1$ for each r (see Lemma 3.1). The eigenvalue $k_{r,n}^2$ of the quantum star graph $(S_N, -\Delta_T)$ is given by*

$$k_{r,n}^2 = \begin{cases}(2n\pi)^2, & \text{if } \alpha_r = 1 \text{ and } n \in \mathbb{N} \text{ with multiplicity } N-1,\\ (2n\pi \pm \frac{\pi}{2})^2, & \text{if } \alpha_r = -i, i \text{ and } n \in \mathbb{N}_0 = \mathbb{N} \cup \{0\},\\ ((2n+1)\pi)^2, & \text{if } \alpha_r = -1 \text{ and } n \in \mathbb{N}_0 = \mathbb{N} \cup \{0\} \text{ with multiplicity } N-1.\end{cases}$$

The eigenvectors of the scattering matrix S associated with α_r are denoted by

$$a_{\alpha_r} = \left(a_1^{\alpha_r}, a_2^{\alpha_r}, ..., a_N^{\alpha_r}, a_{\bar{1}}^{\alpha_r}, a_{\bar{2}}^{\alpha_r}, ..., a_{\bar{N}}^{\alpha_r}\right)^t.$$

The eigenfunction $f_j^{r,n}(x)$ is given as follows:

$$f_j^{r,n}(x) = \begin{cases} C\left(a_j^{\alpha_r} e^{ik_{r,n}x} + a_{\bar{j}}^{\alpha_r} e^{ik_{r,n}(1-x)}\right), & \text{if } \alpha_r \in \{-i, i\},\\ Ca_j^{\alpha_r}\left(e^{i2n\pi x} - e^{i2n\pi(1-x)}\right), & \text{if } \alpha_r = 1,\\ Ca_j^{\alpha_r}\left(e^{i(2n+1)\pi x} + e^{i(2n+1)\pi(1-x)}\right), & \text{if } \alpha_r = -1.\end{cases} \tag{3.7}$$

Proof. Given the star graph S_N with $N \geq 2$, its characteristic polynomial, which is obtained from Theorem 3.4, is

$$K(\alpha) = \left(\alpha^2 + 1\right)(\alpha - 1)^{N-1}(\alpha + 1)^{N-1}.$$

The four eigenvalues are

$$\begin{aligned}&\alpha_1 = 1 \text{ with multiplicity } N-1,\\ &\alpha_2 = i \text{ with multiplicity } 1,\\ &\alpha_3 = -i \text{ with multiplicity } 1, \text{ and}\\ &\alpha_4 = -1 \text{ with multiplicity } N-1.\end{aligned}$$

According to Lemma 3.3, $k^2 = \lambda$ is an eigenvalue of the edge based Laplacian. The eigenvalues are:

$$\begin{array}{ll}(2n\pi)^2 & \text{for every } n \in \mathbb{N} \text{ with multiplicity } N-1,\\ (\pi + 2n\pi)^2 & \text{for every } n \in \mathbb{N}_0 = \mathbb{N} \cup \{0\} \text{ with multiplicity } N-1,\\ \left(\pm\frac{\pi}{2} + 2n\pi\right)^2 & \text{for every } n \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}.\end{array}$$

The eigenfunctions can be obtained by substituting the coefficient values

$$a_1^{\alpha_r}, a_2^{\alpha_r}, ..., a_N^{\alpha_r}, a_{\overline{1}}^{\alpha_r}, a_{\overline{2}}^{\alpha_r}, ..., a_{\overline{N}}^{\alpha_r}$$

from the eigenvector entry a_{α_r} to the solution of the eigenfunctions of the edge-based Laplacian eigenproblem presented in (2.2). $\square$

We can also obtain an eigensystem for the tree $P_2 \rhd S_2$ in a similar way. That is, we first determine the eigenvalues of the scattering matrix for the tree $P_2 \rhd S_2$ and then determine the edge-based Laplacian spectrum using Lemma 3.3. Furthermore, based on (2.2), the Laplacian eigensystem for the tree $P_2 \rhd S_2$ is given in the Corollary below.

Corollary 3.6 (Eigenfunction of the tree $P_2 \rhd S_2$)**.** *As in Lemma 3.3, we denote the eigenvalues of the scattering matrix S by α_r with $|\alpha_r| = 1$ for each r (see Lemma 3.1). The eigenvalue $k_{r,n}^2$ of the quantum tree $(P_2 \rhd S_2, -\Delta_T)$ is given by*

$$k_{r,n}^2 = \begin{cases} (2n\pi)^2, & \text{if } \alpha_r = 1 \text{ and } n \in \mathbb{N}, \\ (2n\pi \pm \arccos(\operatorname{Re}(\alpha_r)))^2, & \text{if } \alpha_r = \pm\left(\frac{1}{3} + i\frac{2}{3}\sqrt{2}\right) \text{ and } n \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}, \\ (2n\pi \pm \arccos(\operatorname{Re}(\alpha_r)))^2, & \text{if } \alpha_r = \pm\left(\frac{1}{3} - i\frac{2}{3}\sqrt{2}\right) \text{ and } n \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}, \\ ((2n+1)\pi)^2, & \text{if } \alpha_r = -1 \text{ and } n \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}. \end{cases}$$

The eigenvectors of the scattering matrix S associated with α_r are given by

$$a_{\alpha_r} = \left(a_1^{\alpha_r}, a_2^{\alpha_r}, ..., a_N^{\alpha_r}, a_{\overline{1}}^{\alpha_r}, a_{\overline{2}}^{\alpha_r}, ..., a_{\overline{N}}^{\alpha_r}\right)^t.$$

The eigenfunction $f_j^{r,n}(x)$ is given as follows:

$$f_j^{r,n}(x) = \begin{cases} C\left(a_j^{\alpha_r} e^{ik_{r,n}x} + a_{\overline{j}}^{\alpha_r} e^{ik_{r,n}(1-x)}\right), & \text{if } \alpha_r = \pm\left(\frac{1}{3} + i\frac{2}{3}\sqrt{2}\right), \\ C\left(a_j^{\alpha_r} e^{ik_{r,n}x} + a_{\overline{j}}^{\alpha_r} e^{ik_{r,n}(1-x)}\right), & \text{if } \alpha_r = \pm\left(\frac{1}{3} - i\frac{2}{3}\sqrt{2}\right), \\ Ca_j^{\alpha_r}\left(e^{i2n\pi x} - e^{i2n\pi(1-x)}\right), & \text{if } \alpha_r = 1, \\ Ca_j^{\alpha_r}\left(e^{i(2n+1)\pi x} + e^{i(2n+1)\pi(1-x)}\right), & \text{if } \alpha_r = -1. \end{cases} \tag{3.8}$$

The steps of the proof are similar to those in Theorem 3.4 and Corollary 3.5. What remains to be shown is that all of the eigenvectors given above completely satisfy the eigenvalue problem (2.1), which is easy to check.

3.3. **The linear wave equation for a quantum tree which has Dirichlet conditions at all leaf vertices.** In this section, we provide a general solution to the wave equation on a tree. The initial condition is a single Gaussian wave packet on an arbitrary edge of the tree.

3.3.1. *Edge-based linear wave equation solution on a tree.* In the following, we present a general solution of the edge-based linear wave equation on a quantum tree obtained using the method of separation of variables and eigenfunctions in (2.2) for the edge-based Laplacian eigenvalue problem.

Proposition 3.7. *Let $\mathcal{X}_j$ be the coordinate on a tree that defines an edge e_j and the standard coordinate value on that edge is x. Let a linear wave equation on the quantum tree $(T_m, -\Delta_T)$ be given as follows:*

$$u_{tt} = \Delta_T u, \qquad t > 0, \text{ and vertex conditions at the vertices of the tree.}$$

The general solution of the linear wave equation is

$$u(\mathcal{X}_j, t) = \sum_k \left[a_j e^{ikx} + a_{\overline{j}} e^{ik(1-x)}\right]\{\alpha_k \cos(kt) + \beta_k \sin(kt)\}, \tag{3.9}$$

where a_j is the coefficient of the eigenfunction on the edge e_j and

$$\{\alpha_k \cos(kt) + \beta_k \sin(kt)\}$$

is the temporal part.

3.3.2. *Initial Conditions.* Since the wave equation is a second-order partial differential equation, we can give the initial conditions and initial velocity,

$$u(\mathcal{X}_j, 0) = p(\mathcal{X}_j) \qquad \text{and} \qquad u_t(\mathcal{X}_j, 0) = r(\mathcal{X}_j).$$

Corollary 3.8. *Given a solution to the linear wave equation in Proposition 3.7. Suppose the initial condition is Gaussian wave packet*

$$p(j,x) = e^{-a(x-\mu)^2}$$

on the edge e_j, zero on the other edges, and the initial velocity is zero. If the value of a is sufficiently large, then the solution to the wave equation is of the form

$$u(\mathcal{X}_j, t) = \sqrt{\frac{\pi}{a}} \sum_k e^{-\frac{k^2}{4a}} \left[a_{j'} e^{ik\mu} + a_{\bar{j}'} e^{ik(1-\mu)}\right] \left[a_j e^{ikx} + a_{\bar{j}} e^{ik(1-x)}\right] \cos(kt),$$

with the value of k is determined by the structure of the quantum tree T.

Proof. We observe that

$$p(\mathcal{X}_j) = \sum_k \left[a_j e^{ikx} + a_{\bar{j}} e^{ik(1-x)}\right] \alpha_k,$$

with

$$\alpha_k = \sum_j F_k,$$
$$F_k = \int_0^1 p(j,x) \left[a_j e^{ikx} + a_{\bar{j}} e^{ik(1-x)}\right] dx.$$

Also, the initial velocity

$$r(\mathcal{X}_j) = \sum_k \left[a_j e^{ikx} + a_{\bar{j}} e^{ik(1-x)}\right] \beta_k k,$$

with

$$\beta_k k = \sum_j G_k,$$
$$G_k = \int_0^1 r(j,x) \left[a_j e^{ikx} + a_{\bar{j}} e^{ik(1-x)}\right] dx.$$

Let the initial condition be a Gaussian wave packet $p(j,x) = e^{-a(x-\mu)^2}$ on a single edge, zero on other edges, and the initial velocity is zero. For a large value of a,

$$\begin{aligned} F_k &= \int_{-\infty}^{\infty} e^{-a(x-\mu)^2} \left[a_j e^{ikx} + a_{\bar{j}} e^{ik(1-x)}\right] dx \\ &= \underbrace{a_j \int_{-\infty}^{\infty} e^{-a(x-\mu)^2} e^{ikx} dx}_{i)} + \underbrace{a_{\bar{j}} \int_{-\infty}^{\infty} e^{-a(x-\mu)^2} e^{ik(1-x)} dx}_{ii)}. \end{aligned}$$

For i),

$$
\begin{aligned}
a_j \int_{-\infty}^{\infty} e^{-a(x-\mu)^2} e^{ikx} dx &= a_j \int_{-\infty}^{\infty} e^{-ax^2+(2\mu a+ik)x-a\mu^2} dx \\
&= a_j \sqrt{\frac{\pi}{a}} e^{\frac{(2\mu a+ik)^2}{4a}-a\mu^2} \\
&= a_j \sqrt{\frac{\pi}{a}} e^{\mu ik-\frac{k^2}{4a}}.
\end{aligned}
$$

For ii),

$$
\begin{aligned}
a_{\bar{j}} \int_{-\infty}^{\infty} e^{-a(x-\mu)^2} e^{ik(1-x)} dx &= a_{\bar{j}} \int_{-\infty}^{\infty} e^{-ax^2+(2\mu a+ik)x-a\mu^2-ikx+ik} dx \\
&= a_{\bar{j}} \sqrt{\frac{\pi}{a}} e^{\frac{(2\mu a+ik)^2}{4a}-a\mu^2+ik} \\
&= a_{\bar{j}} \sqrt{\frac{\pi}{a}} e^{(1-\mu)ik-\frac{k^2}{4a}}.
\end{aligned}
$$

From $i)$ and $ii)$, we obtain

$$
F_k = \sqrt{\frac{\pi}{a}} e^{-\frac{k^2}{4a}} \left[a_j e^{ik\mu} + a_{\bar{j}} e^{ik(1-\mu)} \right].
$$

Since $r(\mathcal{X}_j) = 0$, it follows that $\beta_k = 0$. □

3.3.3. *A particular form of the solution of the wave equation.* For some particular value of k, we can calculate

$$
u_k(\mathcal{X}_j, t) = \sqrt{\frac{\pi}{a}} e^{-\frac{k^2}{4a}} \left[a_{j'} e^{ik\mu} + a_{\bar{j}'} e^{ik(1-\mu)} \right] \left[a_j e^{ikx} + a_{\bar{j}} e^{ik(1-x)} \right] \cos(kt). \tag{3.10}
$$

From this equation, the solution to the wave equation on a quantum tree with Dirichlet conditions at the leaf vertex can be obtained from superposition of several equations depending on a particular structure of the tree.

Theorem 3.9. *Consider the eigenfunctions in (3.7) and (3.8) obtained from the Laplacian eigenvalue problem on the quantum trees S_N and $P_2 \rhd S_2$, respectively. Then, the particular form of the solution of the wave equation on the quantum tree S_N and $P_2 \rhd S_2$ (3.10) for some frequency k is given as follows:*

(1) $u_{2n\pi} = \sqrt{\frac{\pi}{a}} \sum_n e^{-\frac{(2n\pi)^2}{4a}} \left[a_{j'} \left(e^{2n\pi i\mu} - e^{2n\pi i(1-\mu)} \right) \right] \times$
$\left[a_j \left(e^{2n\pi ix} - e^{2n\pi i(1-x)} \right) \right] \cos(2n\pi t)$ *for* $k = 2n\pi$.

(2) $u_{(2n+1)\pi} = \sqrt{\frac{\pi}{a}} \sum_n e^{-\frac{(2n+1)^2\pi^2}{4a}} \left[a_{j'} \left(e^{(2n+1)\pi i\mu} + e^{(2n+1)\pi i(1-\mu)} \right) \right] \times$
$\left[a_j \left(e^{(2n+1)\pi ix} + e^{(2n+1)\pi i(1-x)} \right) \right] \cos((2n+1)\pi t)$ *for* $k = (2n+1)\pi$.

(3) $u_{k_p} = \sqrt{\frac{\pi}{a}} \sum_{k_p} e^{-\frac{k_p^2}{4a}} \left[a_{j'} e^{ik_p\mu} + a_{\bar{j}'} e^{ik_p(1-\mu)} \right] \left[a_j e^{ik_px} + a_{\bar{j}} e^{ik_p(1-x)} \right] \times$
$\cos(k_pt)$ *for* $k_p = 2n\pi \pm \arccos(\mathrm{Re}(\alpha_r))$.

The above theorem directly follows from of (3.10) for both types of the trees (the star graph S_N and $P_2 \rhd S_2$). We skip the formal proof. The formula given is evident, and all the eigenfunctions used have appeared in Corollaries 3.5 and 3.6. The computational part of the proof that (1)—(3) in Theorem 3.9 satisfy the linear wave equation is straightforward.

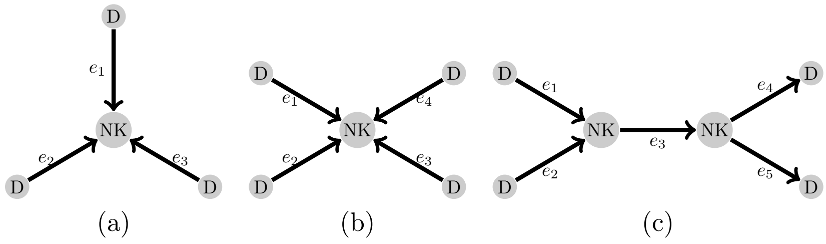

FIGURE 3. (a) Quantum star graph S_3, (b) quantum star graph S_4, and (c) quantum tree $P_2 \rhd S_2$. (The letters D, NK signify the Dirichlet, and Neumann-Kirchhoff vertex conditions, respectively. Where the direction of the edge e is determined by a parameter ranging from 0 to 1).

4. SIMULATION

In this section, we present a simulation of the evolution of a wave traveling through an edge per unit of time t. Simulations are performed on the star graphs S_3, S_4 and the quantum tree $P_2 \rhd S_2$ with the initial conditions of Gaussian wave packets starting on the edge e_1. Figure 3 presents the quantum trees that will be used in the simulation.

We obtain a simulation of wave evolution by implementing the exact solutions from Theorem 3.9. The tree structure affects the calculation of the frequency values k. We refer to Corollaries 3.5 and 3.6 to get the frequency values k.

We present the wave evolution simulation in a heatmap diagram which expresses the amplitude of the wave propagating at the edge per unit of time. The different colors represent the amplitude values at a certain edge and time. This data set is obtained from the amplitude value of the exact solution of the wave equation at the edge per unit of time. A more illustrative and physical diagram of the wave evolution is given for the star graph S_3 (Figure 4).

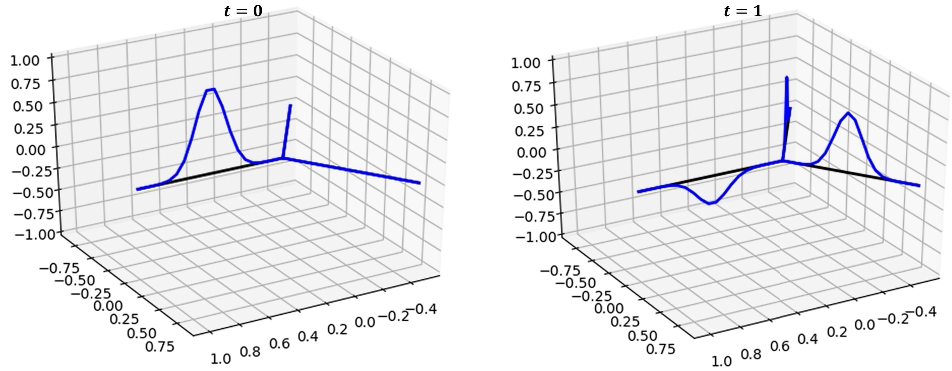

FIGURE 4. The solution of the wave equation on the star graph S_3 at time $t = 0$ and $t = 1$

Figure 4 a simulation of the wave solution with the Gaussian wave packet as the initial condition at the edge e_1 and time $t = 0$ with the value of the amplitude equal to 1. Furthermore, a_1 represents the wave amplitude that propagates in the direction to the interior vertex on edge e_1. Figure 5 (a) presents a heatmap diagram for the wave evolution on the star graph S_3. The amplitude of the Gaussian packet wave propagating in the direction to the interior vertex is represented by a_1, a_2, a_3 and the opposite direction is represented by $a_{\bar{1}}$, $a_{\bar{2}}$, and $a_{\bar{3}}$ for $t = 0 \ldots 4$. The amplitude of the waves due to scattering at $t = 1$ is the amplitude of $a_{\bar{1}}$ of $-1/3$ (reflection occurs) and the amplitude of a_2, a_3 of $2/3$ (transmission occurs).

Furthermore, Figure 5 (b) provides a heatmap diagram for simulating the wave evolution on the star graph S_4. In this case, the scattering that occurs at $t = 1$ produces one wave (reflection) with an amplitude value of $a_{\bar{1}}$ is $-1/2$ and three waves (transmission occurs) with an amplitude value of a_2, a_3, a_4 is $1/2$.

Finally, Figure 5 (c) presents a heatmap diagram for simulating the evolution of waves propagating for the tree $P_2 \triangleright S_2$. Starting with the initial conditions on the edge e_1 with the amplitude value of a_1, it propagates towards the interior vertex. There are many scattering occurs so that one can see the difference in the amplitude values generated at each edge. Next, Figure 5 (d) presents a heatmap diagram of the wave amplitude data on the edges of the tree $P_2 \triangleright S_2$. In this diagram, each edge e_j represents the sum of the wave amplitude values a_j and $a_{\bar{j}}$ per unit of time. So the diagram in Figure 4 (d) only presents the wave amplitude at an edge per unit of time regardless of the direction of the wave propagation.

Since the initial condition is the amplitude of the Gaussian packet wave represented a_1 at edge e_1. The wave propagation can be seen from end to end with the initial condition that the Gaussian wave amplitude is at the end of e_1. Scattering occurs at $t = 1$ because a wave with an amplitude of a_1 meets the interior vertex. Then a negative amplitude is generated due to reflection at the leaf vertices with the Dirichlet condition at $t = 2$ at the edge of e_1. We present all heatmap diagrams that give the amplitude values of the waves propagating in the quantum tree in Figure 5.

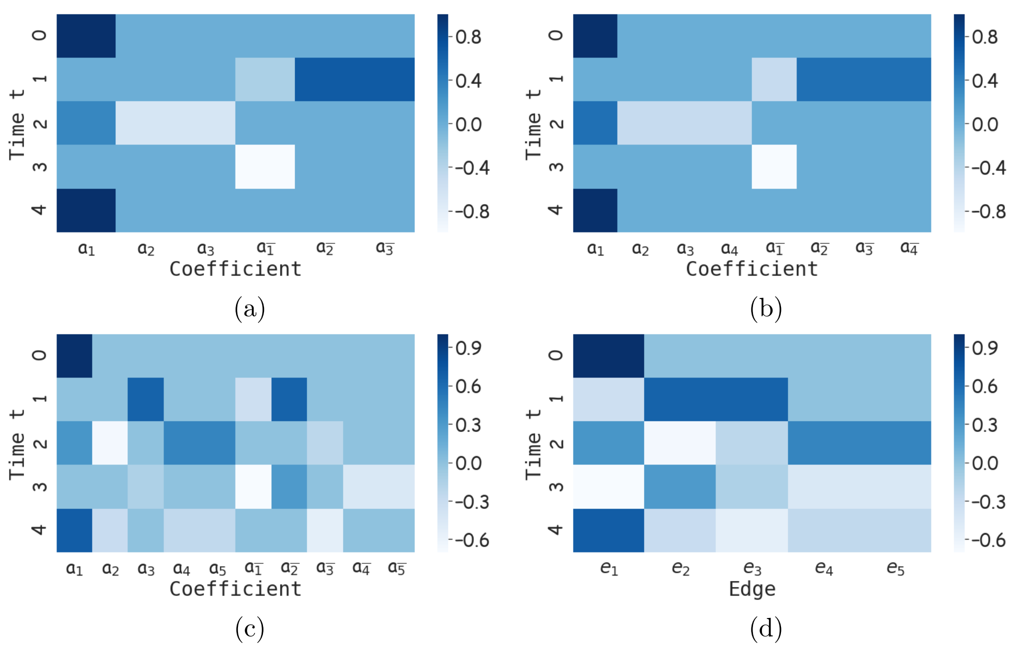

FIGURE 5. The amplitudes of the Gaussian wave packet evolution on (a) the star graph S_3, (b) the star graph S_4, (c) and (d) the tree $P_2 \triangleright S_2$ with t ranging from 1 to 4 units of time.

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