Thermal diffusion in branched structures: Metric graph based approach

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We consider the problem of heat diffusion in branched systems and networks on the basis of a model described in terms of the heat equation on metric graphs. Using the explicit analytical solutions of the latter, evolution of the temperature profile and heat flow on each branch are computed. Extension of the study for nonlinear regime is considered using a nonlinear heat equation on metric graphs. It is found that in nonlinear regime is more intensive than that in linear case.

1. INTRODUCTION

Particle and wave transport in low dimensional branched structures is of importance for different technological applications. Discrete structures, networks and other types of branched systems appear as part of many materials and devices at macro-, micro- and even nanoscale. Tuning, optimization and controlling functionality of such devices require deep understanding of wave phenomena in such branched structures and effective, maximally realistic modeling of these phenomena. The latter requires using simple and powerful approaches for such modeling. One of such approaches is based on the use of different wave (partial differential) equation on so called metric graphs. The graph itself is determined as a set of bonds connected to each other at the vertices (branching points) according to some rule which is called the topology of a graph. When bonds of a graph are assigned length it is called metric graph. Topology of a graph is given in terms of the adjacency matrix which can be written as [1, 4]:

\[ C_{ij} = C_{ji} = \begin{cases} 
1 & \text{if } i \text{ and } j \text{ are connected,} \\
0 & \text{otherwise,} 
\end{cases} \quad (1.1) \]

\( i, j = 1, 2, ..., V. \)

Study of wave dynamics in branched systems using metric graphs can be divided into two cases: transport of the waves in linear and nonlinear regimes. Investigation of the linear waves in branched systems are focused mainly on so-called "quantum graphs" which are described in terms of linear Schrödinger equation on metric graphs. Pioneering treatments of quantum mechanical motion in branched systems has been considered few decades ago in the Refs. [7]-[9]. However, strict treatment of quantum graphs was first presented by Exner, Seba and Stovicek to describe free quantum motion on branched wires [10]. Later Kostrykin and Schrader derived the general boundary conditions providing self-adjointness of the Schrödinger operator on graphs [11]. Toth and Harrison extended such conditions for the Dirac operator on metric graphs [12]. Hul et al considered experimental realization of quantum graphs in optical microwave networks [2]. An important topic related to quantum graphs was studied in the context of quantum chaos theory and spectral statistics [1, 4, 12–14]. Spectral properties and band structure of periodic quantum graphs also attracted much interest [15, 16]. Different aspects of the Schrödinger operators on graphs have been studied in the Refs. [6, 17–20, 21]. Despite great progress made on the study of quantum graphs, other wave equations on metric graphs are still remaining out of the focus, although some mathematical aspects of partial differential equations on graphs have been considered in the literature (see, e.g., [22]-[31]). Nonlinear wave dynamics in branched systems which are described by nonlinear evolution equations on metric graphs has attracted much attention during past decade [31–40].

In this paper we consider dynamics of thermal waves in branched systems which are modeled in terms of the linear and nonlinear heat equations on metric graphs. Such a model can be used for describing the classical (non-quantum) heat diffusion in branched polymers, carbon nanotube networks and any low-dimensional branched structures appearing in condensed matter physics.

FIG. 1: Metric star graph. \( L_j \) is the length of the \( j \)th bond with \( j = 1, 2, 3. \)

2. LINEAR HEAT DIFFUSION IN NETWORKS

Our aim is modeling the heat diffusion in branched structures using heat equation on metric graphs. Solution of the latter can be constructed using that of heat equation on a finite interval, (0; \( l \)) which is given by [41-44].
where \( u(x,t) \) is the temperature profile, \( \kappa \) is the heat conductivity. The boundary and initial conditions are imposed as
\[
    u(0,t) = u(t,0) = 0, \quad u(x,0) = f(x), \tag{2.2, 2.3}
\]

Exact solutions of the problem (2.1)-(2.3) can be obtained by separating variables as
\[
    u(x,t) = X(x)T(t), \tag{2.4}
\]
that gives the general solution of Eq. (2.1)
\[
    u(x,t) = \sum_{n=1}^{\infty} C_n e^{-\frac{\kappa^2 \pi^2}{L^2} n^2 \sin \left( \frac{n \pi}{l} \right)} \tag{2.5}
\]

In the following this solution will be used to construct the solution of the heat equation on metric graphs with finite bonds. We note that mathematical aspects of the heat equation on graphs have been earlier considered in the Refs. [24, 31]. Here we will obtain explicit solution of heat equation on metric graph and apply it for modeling heat diffusion in networks.

Consider the star graph consisting of three bonds \( b_j (j = 1, 2, 3) \) with the lengths \( L_j (j = 1, 2, 3) \) connected at one vertex (See, Fig. 1). On each bond of this graph we have heat equation given by
\[
    \frac{\partial u_j}{\partial t} = \kappa_j^2 \frac{\partial^2 u_j}{\partial x^2}, \tag{2.6}
\]
with \( \kappa_j \) being the heat conductivity of each branch of the graph. Initial condition for Eq. (2.6) can be imposed as
\[
    u_j(x,0) = f_j(x). \tag{2.7}
\]

To solve Eq. (2.6), one needs to impose also the boundary conditions at the branching point (vertex) of graph and at the bond edges. At the bonds edges we can impose Dirichlet boundary conditions given by
\[
    u_j(L_j) = 0, \tag{2.8}
\]
while the vertex boundary conditions can be imposed as
\[
    u_1(0,t) = u_2(0,t) = u_3(0,t) \tag{2.9}
\]
\[
\frac{\partial u_1}{\partial x} + \frac{\partial u_2}{\partial x} + \frac{\partial u_3}{\partial x} \bigg|_{x=0} = 0. \tag{2.10}
\]

Eq. (2.10) is the continuity of solution at the vertex, while Eq. (2.11) provides Kirchhoff rule for the heat flux. Using the prescription, proposed in [11], one can easily make sure that these boundary conditions provide self-adjointness of the heat equation on a graph.

Variables in Eq. (2.6) can be separated by the substitution
\[
    u_j(x,t) = X_j(x)T(t), j = 1, 2, 3, \tag{2.11}
\]
that gives rise to equations
\[
    X_j''(x) + \frac{\lambda^2}{\kappa_j^2} X_j(x) = 0, \tag{2.12}
\]
presents evolution of the temperature profile, can be written as

\[ u_j(x, t) = \sum_{n=1}^{\infty} a_n^{(j)} e^{-\lambda_n^2 t} \frac{\lambda_n}{\kappa_j} (x - L_j). \]  \hfill (2.18)

where \( a_n^{(j)} = \int_0^{L_j} f_j(x) \frac{\lambda_n}{\kappa_j} (x - L_j) dx. \)

existence of the roots of Eq. (2.17) (which can be easily shown, e.g., using the Newton’s method) implies solvability of Eq. (2.17) on metric graph. Therefore finding numerically the roots of Eq. (2.17) one can construct complete set of eigenvalues of the problem given by Eqs. (2.6) - (2.10).

Then the general solution of the heat equation on metric star graph, which describes evolution of the temperature profile, can be written as

\[ u_j(x, t) = \sum_{n=1}^{\infty} a_n^{(j)} e^{-\lambda_n^2 t} \frac{\lambda_n}{\kappa_j} (x - L_j). \]  \hfill (2.18)

where \( a_n^{(j)} = \int_0^{L_j} f_j(x) \frac{\lambda_n}{\kappa_j} (x - L_j) dx. \)

Fig. 2 provides evolution of the temperature profile in metric star graph calculated using the solution of Eq. (2.18) for the values of heat conductivity \( \kappa_1 = 0.3, \kappa_2 = 0.5, \kappa_3 = 0.7 \) and bond lengths \( L_1 = 10, L_2 = 11, L_3 = 12 \). The initial condition, i.e. the temperature profile at \( t = 0 \) is chosen as \( f_j(x) = \text{sech}(x) \). An important characteristics of the heat diffusion is the heat flux determined as \( Q_j(x, t) = -\kappa_j \frac{\partial u_j}{\partial x} \) . Fig. 3 presents plots of the heat flux vs coordinate and time on each bond of a star graph for the values of heat conductivity \( \kappa_1 = 4.5, \kappa_2 = 8, \kappa_3 = 8.4 \) and for the same initial condition and bond lengths as those in Fig. 2.

3. EXTENSION TO OTHER GRAPHS

The above treatment can be easily extended to other graph topologies, such as tree and loop graphs. The tree graph (see Fig. 4) consists of three subgraphs \( b_1, (b_{1i}), (b_{1ij}), \) where \( i, j \) run over the given bonds of a subgraph. On each bond \( b_1, b_{1i}, b_{1ij} \) we have heat equation given by

\[ \frac{\partial u_b}{\partial t} = \kappa_b \frac{\partial^2 u_b}{\partial x^2}, \ k_b > 0 \]  \hfill (3.1)

for which the initial and boundary conditions can be written as

\[ u_b(x, 0) = f_b(x), 0 < x < L_b, \]  \hfill (3.2)

\[ u_1(0, t) = 0, u_{1ij}(L_{1ij}, t) = 0, i = 1, 2, j = 1, 2 \]  \hfill (3.3)
plotted using the solution of the problem (4.1)-(4.2) for

\[ \beta_1 = 1, \beta_2 = \sqrt{2}, \beta_3 = \sqrt{2} \text{ and } L_1 = L_2 = L_3 = 2. \]

\[ u_1(L_1, t) = u_{1i}(0, t), i = 1, 2 \] (3.4)

\[ u_{1i}(L_{1i}, t) = u_{1ij}(0, t), i = 1, 2; j = 1, 2 \] (3.5)

\[ \frac{\partial u_1}{\partial x} \bigg|_{x=L_1} - \sum_{i=1}^{2} \frac{\partial u_{1i}}{\partial x} \bigg|_{x=0} = 0, i = 1, 2 \] (3.6)

\[ \frac{\partial u_{1i}}{\partial x} \bigg|_{x=L_{1i}} - \sum_{j=1}^{2} \frac{\partial u_{1ij}}{\partial x} \bigg|_{x=0} = 0, i = 1, 2. \] (3.7)

Variables in Eq. (3.11) can be separated and we get from the boundary conditions, the secular equation for finding the eigenvalues, \( \lambda_n \), that allows to obtain the complete set of the eigenvalues and eigenfunctions similarly to that for the star graph.

For the loop graph presented in Fig. 5 we have

\[ \frac{\partial}{\partial x} u_j = \kappa_j \frac{\partial^2}{\partial x^2} u_j, \kappa_j > 0 \] (3.8)

\[ u_j(x, 0) = f_j(x) \] (3.9)

\[ u_1(0, t) = u_4(L_4, t) = 0 \] (3.10)

\[ u_1(L_1, t) = u_2(0, t) = u_3(0, t) \] (3.11)

\[ u_2(L_2, t) = u_3(L_3, t) = u_4(0, t) \] (3.12)

\[ \frac{\partial u_1}{\partial x} \bigg|_{x=L_1} - \frac{\partial u_2}{\partial x} \bigg|_{x=0} - \frac{\partial u_3}{\partial x} \bigg|_{x=0} = 0. \] (3.13)

\[ \frac{\partial u_2}{\partial x} \bigg|_{x=L_2} + \frac{\partial u_3}{\partial x} \bigg|_{x=L_3} - \frac{\partial u_4}{\partial x} \bigg|_{x=0} = 0. \] (3.14)

Separating variables by substitution \( 2.11 \) we get Eqs. \( 2.12 \) and \( 2.13 \) with the boundary conditions given by

\[ X_1(0) = X_4(L_4) = 0. \] (3.15)

\[ X_1(L_1) = X_2(0) = X_3(0). \] (3.16)

\[ X_2(L_2) = X_3(L_3) = X_4(0). \] (3.17)

\[ X_1'(x)|_{x=L_1} - X_2'(x)|_{x=0} - X_3'(x)|_{x=0} = 0. \] (3.18)

\[ X_2'(x)|_{x=L_2} + X_3'(x)|_{x=L_3} - X_4'(x)|_{x=0} = 0. \] (3.19)

General solution can be written as

\[ X_j(x) = A_j \cos \frac{\lambda_j}{\kappa_j}(x-L_j) + B_j \sin \frac{\lambda_j}{\kappa_j}(x-L_j), j = 1, 2, 3, 4 \]

After some algebra we get the following system of equations from which we can find \( \lambda_n, A_j \) and \( B_j \):

\[ B_1 \sin \frac{\lambda}{\kappa_1}L_1 - A_2 \cos \frac{\lambda}{\kappa_2}L_2 - B_2 \sin \frac{\lambda}{\kappa_2}L_2 = 0 \]

\[ B_1 \sin \frac{\lambda}{\kappa_1}L_1 - A_3 \cos \frac{\lambda}{\kappa_3}L_3 - B_3 \sin \frac{\lambda}{\kappa_3}L_3 = 0 \]

\[ A_2 - A_3 = 0 \]

\[ A_2 + B_4 \sin \frac{\lambda}{\kappa_4}L_4 = 0 \]

\[ \frac{\lambda}{\kappa_1}B_1 \cos \frac{\lambda}{\kappa_1}L_1 - \frac{\lambda}{\kappa_2}A_2 \sin \frac{\lambda}{\kappa_2}L_2 - \frac{\lambda}{\kappa_2}B_2 \cos \frac{\lambda}{\kappa_2}L_2 - \frac{\lambda}{\kappa_3}A_3 \sin \frac{\lambda}{\kappa_3}L_3 - \frac{\lambda}{\kappa_3}B_3 \cos \frac{\lambda}{\kappa_3}L_3 = 0 \]

\[ \frac{\lambda}{\kappa_2}B_2 + \frac{\lambda}{\kappa_3}B_3 - \frac{\lambda}{\kappa_4}B_4 \cos \frac{\lambda}{\kappa_4}L_4 = 0 \]

Eigenvalues, eigenfunctions and general solutions can be found similarly to those for star and tree graphs.
4. HEAT DIFFUSION IN NONLINEAR REGIME

The above model for the linear heat diffusion in networks can be extended to the case of nonlinear regime, using a nonlinear heat equation on metric graph. Here we demonstrate it for a star graph with three semi-infinite bonds. Consider the following nonlinear heat equation on a star graph with the bonds $b_1 \sim (-\infty;0)$, $b_{2,3} \sim (0;+\infty)$:

$$\frac{\partial u_j}{\partial t} - \frac{\partial^2 u_j}{\partial x^2} = -2\beta_j^2 u_j^3, \ x \in b_j, \ t > 0 \quad (4.1)$$

for which the vertex boundary conditions are imposed as

$$\beta_1 u_1(0,t) = \beta_2 u_2(0,t) = \beta_3 u_3(0,t),$$

$$\left. \frac{1}{\beta_1} \frac{\partial u_1}{\partial x} \right|_{x=0} = \left. \frac{1}{\beta_2} \frac{\partial u_2}{\partial x} \right|_{x=0} + \left. \frac{1}{\beta_3} \frac{\partial u_3}{\partial x} \right|_{x=0}. \quad (4.2)$$

Solution of the equation (4.1) (without boundary conditions) can be written as

$$u_j(x,t) = \frac{x-x_0}{\beta_j} \left( (x-x_0)^2 + 6t \frac{1}{\sqrt{2}} \right). \quad (4.3)$$

Fulfilling the boundary conditions (4.2) by this solution is possible if coefficients $\beta_j, \ j=1, 2, 3$ obey the following (constraints) sum rule:

$$\frac{1}{\beta_1^2} = \frac{1}{\beta_2^2} + \frac{1}{\beta_3^2}. \quad (4.4)$$

Eq. (4.4) presents the condition for integrability of nonlinear heat equation on metric star graph. Fig. 7 presents evolution of the temperature profile plotted using Eq. (4.3) for the case when the sum rule given by Eq. (4.4) is fulfilled. Corresponding plot of the heat flux on each bond is presented in Fig. 8. Comparing the plots of the heat flux with those for linear case we can conclude that in nonlinear regime heat flux is more intensive than that in linear one.

5. CONCLUSIONS

We studied heat diffusion on branched systems by considering linear and nonlinear regimes of diffusion. Exact analytical solutions of linear heat equation on simple metric graphs are obtained. Temperature profiles for such systems are computed. Nonlinear regime is studied on the basis of a nonlinear heat equation on metric star graph. Exact solutions are obtained for the case, when nonlinearity coefficient fulfills some constraint which can be written in the form of sum rule. The above models can be applied for the study of linear and nonlinear heat diffusion in different branched materials such as polymers, carbon nanotube networks, DNA and different low-dimensional networks.

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