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Time dependent quantum graph with loop

D. A. Eremin[1], E. N. Grishanov[1], O. G. Kostrov[1], D. S. Nikiforov[2], I. Y. Popov[2]

[1]Department of Mathematics and IT, Ogarev Mordovia State University
Bolshevistskaya Str. 68, Saransk, Russia

[2]Department of Higher Mathematics, ITMO University, Kroverkskiy pr. 49, St. Petersburg, 197101, Russia

popov1955@gmail.com

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A quantum graph, consisting of a ring and segment is considered. We deal with the free Schrödinger ooperator at the edges and Kirchhoff conditions at the internal vertex. The lengths of the graph edges varies in time. Time evolution of wave packet is studied for different parameters of length varying law.

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1. Introduction

A quantum graph is a rather old mathematical model introduced initially to aid in the description of macromolecules [1]. Later, it was used in many problems of quantum theory. In spite of its simplicity, the model gives one a powerful instrument for investigating quantum systems. As for rigorous mathematical models of such type, they appeared in the 80's [2]. The mathematical background of the approach is the theory of self-adjoint operator extensions (see, e.g., [3, 4] and references in [5]) related to model of point-like potentials in quantum physics. There are a large number of works in the field (see, e.g., [6–9] and references therein).

The problem of time-dependent boundary conditions in the Schrödinger equation has attracted much attention in the context of quantum Fermi acceleration [10]. A detailed study of the problem can be found in [11]. In particular, it was pointed out that the problem of 1D box with a moving wall can be mapped onto that of an harmonic oscillator with time-dependent frequency confined inside the static box. Time-dependent point-like potentials and related topics of the operator extensions theory were studied in several works (see, e.g., [12] and references therein). Star-like quantum graphs having edges with time varying lengths have been discussed [13]. Problems concerning the boundary conditions for time-depended interval are discussed in [14].

In the present paper, we consider simple quantum graph with a loop (see Fig. 1). The lengths of edges vary in time. We construct a mathematical model and investigate the time evolution of initial wave packet.

2. The description of the model

2.1. Stationary problem

To describe the system evolution, we start from the stationary problem. The quantum graph is determined in a conventional way. The Hamiltonian is the free Schrödinger operator, i.e. $-\dfrac{d^2}{dy^2}$, at each edge and the Kircchoff conditions at the internal vertex of the graph. The length of the segment is assumed to be 1, the circle radius is r. Let us mark the electron wave function as ϕ_ℓ at the segment and as ϕ_r at the ring. Then, one has the following equation at each edge:

$$-\frac{d^2}{dy^2}\phi_\ell(y) = k^2\phi_\ell(y), 0 \le y \le 1,$$

$$-\frac{d^2}{dy^2}\phi_r(y) = k^2\phi_r(y), 0 \le y \le 2\pi r,$$

$$\begin{cases} \phi_\ell(0) = \phi_r(0) = \phi_r(2\pi r), \\ \phi_\ell(\ell) = 0, \\ \dfrac{d}{dy}\phi_l|_{y=0} + \dfrac{d}{dy}\phi_r|_{y=0} - \dfrac{d}{dy}\phi_r|_{y=2\pi r} = 0. \end{cases}$$

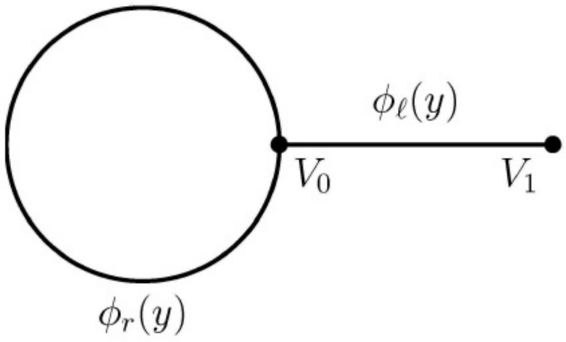

FIG. 1. Graph geometry

As for the boundary vertex of the graph, we assume here Dirichlet conditions. Eigenfunctions take the form:

$$\phi_\ell^{(n)}(y) = \frac{1}{B_n}\frac{\sin(k_n(1-y))}{\sin(k_n)},$$
$$\phi_r^{(n)}(y) = \frac{1}{B_n}\frac{\cos\left(k_n(y-\pi r)\right)}{\cos\left(k_n\pi r\right)},$$

where k_n is the $n-$th positive root of the spectral equation having the form:

$$2\tan\left(\pi kr\right) = \cot k.$$

B_n is the normalizing constant:

$$B_n^2 = \frac{1}{2\sin^2(k_n)} + \frac{\pi r}{\cos^2(\pi k_n r)}.$$

2.2. Non-stationary problem

Let us consider a non-stationary graph. We assume that the edge lengths vary with time, $L_\ell = L(t)$, $L_r = 2\pi r L(t)$. Here, $L(t)$ is a smooth positive function (we will choose it later). In this case, the particle dynamics in graph are described by the following time-dependent Schrödinger equation:

$$\imath\frac{\partial}{\partial t}\Psi_\ell(x,t) = -\frac{\partial^2}{\partial x^2}\Psi_\ell(x,t), 0 \le x \le L(t),$$
$$\imath\frac{\partial}{\partial t}\Psi_r(x,t) = -\frac{\partial^2}{\partial x^2}\Psi_r(x,t), 0 \le x \le 2\pi r L(t),$$

for the time-dependent wave function:

$$\Psi(t) = \begin{pmatrix} \Psi_\ell(x,t) \\ \Psi_r(x,t) \end{pmatrix}.$$

Here, the first argument of $\Psi_\ell(x,t)$ varies as follows $0 \le x \le L(t)$ and the first argument of $\Psi_r(x,t)$ – in $0 \le x \le 2\pi r L(t)$. We choose the system of units in which the Planck's constant, speed of light and the electron mass are as follows: $\hbar = c = 1$, $m = 1/2$. The following coupling conditions (Kircchoff conditions) take place at the internal vertex V_0 of the graph and the Dirichlet condition at vertex V_1:

$$\begin{cases} \Psi_\ell|_{x=0} = \Psi_r|_{\varphi=0} = \Psi_r|_{\varphi=2\pi r}, \\ \Psi_\ell(L(t)) = 0, \\ \dfrac{\partial}{\partial x}\Psi_\ell|_{x=0} + \dfrac{\partial}{\partial x}\Psi_r|_{x=0} - \dfrac{\partial}{\partial x}\Psi_r|_{x=2\pi r} = 0. \end{cases} \tag{1}$$

Let us replace the variables at the edges: $y = \dfrac{x}{L(t)}$. Then, the equations change (we have the same equation both at the segment and at the ring, they differ only in variables range):

$$\imath\frac{\partial}{\partial t}\Psi_\ell(y,t) = -\frac{1}{L^2(t)}\frac{\partial^2}{\partial y^2}\Psi_\ell(y,t) + \imath\frac{\dot{L}(t)}{L(t)}y\frac{\partial}{\partial y}\Psi_\ell(y,t), \quad 0 \le y \le 1,$$
$$\imath\frac{\partial}{\partial t}\Psi_r(y,t) = -\frac{1}{L^2(t)}\frac{\partial^2}{\partial y^2}\Psi_r(y,t) + \imath\frac{\dot{L}(t)}{L(t)}y\frac{\partial}{\partial y}\Psi_r(y,t), \quad 0 \le y \le 2\pi r.$$

To obtain a self-adjoint problem, we make the following replacement:

$$\Psi(t) = \begin{pmatrix} \Psi_\ell(y,t) \\ \Psi_r(y,t) \end{pmatrix} = \frac{1}{\sqrt{L(t)}} e^{\imath \frac{L\dot{L}}{4} y^2} \begin{pmatrix} \psi_\ell(y,t) \\ \psi_r(y,t) \end{pmatrix}.$$

Correspondingly, one has the following equations for functions $\psi_\ell(y,t), \psi_r(y,t)$:

$$\begin{aligned} \imath \frac{\partial}{\partial t}\psi_\ell(y,t) &= -\frac{1}{L^2(t)}\frac{\partial^2}{\partial y^2}\psi_\ell(y,t) + \frac{L\ddot{L}}{4} y^2 \psi_\ell(y,t), \quad 0 \le y \le 1, \\ \imath \frac{\partial}{\partial t}\psi_r(y,t) &= -\frac{1}{L^2(t)}\frac{\partial^2}{\partial y^2}\psi_r(y,t) + \frac{L\ddot{L}}{4} y^2 \psi_\ell(y,t), \quad 0 \le y \le 2\pi r. \end{aligned} \tag{2}$$

One can see that the Kirchoff conditions (1) remain for functions $\psi_\ell(y,t), \psi_r(y,t)$ at vertex V_0 and the Dirichlet conditions at V_1.

Taking into account that now the geometric graph is stationary after the chang of variables, we use the expansions with respect to complete system of orthogonal and normalized eigenfunctions of the self-adjoint operator (see Section 2):

$$\begin{pmatrix} \psi_\ell(y,t) \\ \psi_r(y,t) \end{pmatrix} = \sum_n C_n(t) \begin{pmatrix} \phi_\ell^{(n)}(y) \\ \phi_r^{(n)}(y) \end{pmatrix}. \tag{3}$$

Let us insert (3) into (2) and (3). We obtain the system for coefficients C_n:

$$\imath \dot{C}_m(t) = -\frac{k_m^2}{L^2} C_m(t) + \sum_n M_{mn} C_n(t), \tag{4}$$

where:

$$M_{mn} = \frac{L\ddot{L}}{4} \left(\int_0^1 y^2 \phi_\ell^{(n)}(y) \overline{\phi_\ell^{(m)}(y)} dy + \int_0^{2\pi r} y^2 \phi_r^{(n)}(y) \overline{\phi_r^{(m)}(y)} dy \right). \tag{5}$$

This is an infinite system. We truncate it and numerically solve the obtained finite-size system. To consider the evolution of wave packet, we realize the following procedure: we take some initial value for the wave function, expand it in a series, truncate the series, solve the system for coefficients and summarize the series with coefficients corresponding to chosen time value. Correspondingly, we choose the initial condition:

$$\Psi(0) = \begin{pmatrix} \Psi_l(x,0) \\ \Psi_r(x,0) \end{pmatrix}.$$

The initial values for $\psi_\ell(y,t), \psi_r(y,t)$ are obtained in the following way:

$$\begin{pmatrix} \psi_\ell(y,0) \\ \psi_r(y,0) \end{pmatrix} = \begin{pmatrix} L(0) e^{-\imath \frac{L(0)\dot{L}(0)}{4} y^2} \Psi_\ell(y,0) \\ 0 \end{pmatrix}.$$

Correspondingly, the initial values for our system of ordinary differential equation are as follows:

$$C_n(0) = \int_0^1 \psi_\ell(y,0) \overline{\phi_\ell^{(n)}} dy. \tag{6}$$

The solution of the system (4) gives us values for $C_n(t)$. By inserting it into (3), we obtain the wave function for the moment t.

3. Results and discussion

We will choose the particular type of length variation, namely, the harmonic dependence:

$$L(t) = a + b\cos(\omega t). \tag{7}$$

Here, ω is the frequency of the length vibration. We take the following initial wave function (concentrated at the segment):

$$\Psi(0) = \begin{pmatrix} \Psi_l(x,0) \\ \Psi_r(x,0) \end{pmatrix} = \begin{pmatrix} (1-\cos(2\pi x))\sqrt{2/3} \\ 0 \end{pmatrix}.$$

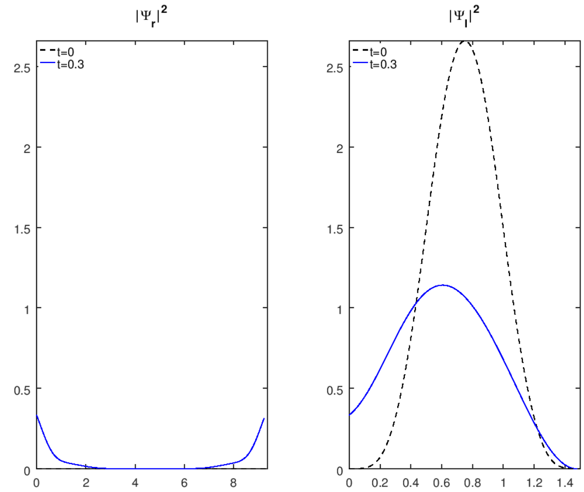

FIG. 2. The wave function at the ring (left) and segment (right) $t = 0$, $t = 0.3$ (arbitrary units)

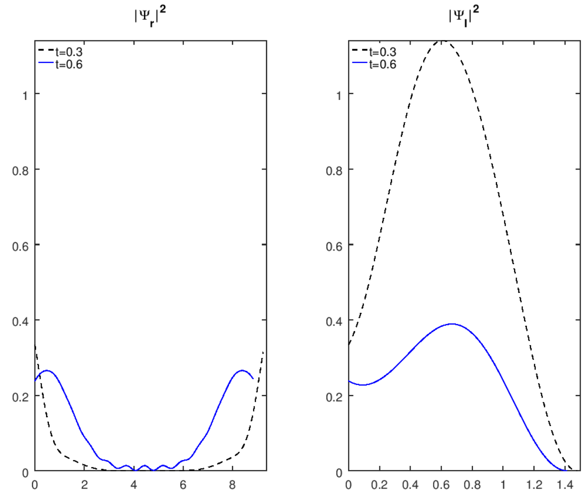

FIG. 3. The wave function at the ring (left) and segment (right) $t = 0.3$, $t = 0.6$ (arbitrary units)

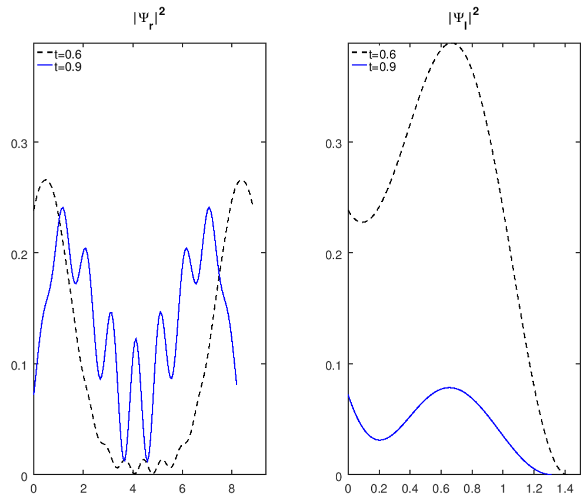

FIG. 4. The wave function at the ring (left) and segment (right) $t = 0.6$, $t = 0.9$ (arbitrary units)

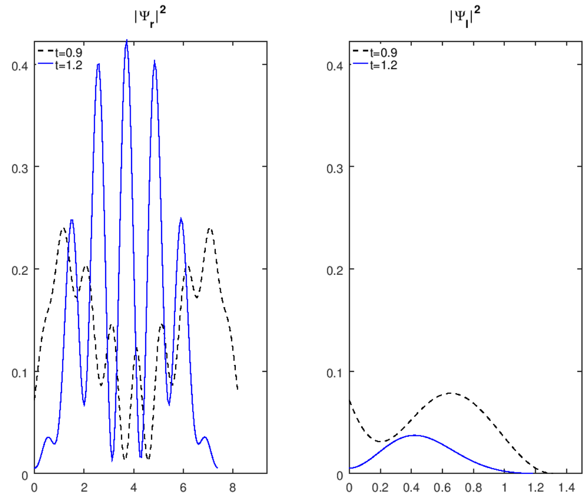

FIG. 5. The wave function at the ring (left) and segment (right) $t = 0.9$, $t = 1.2$ (arbitrary units)

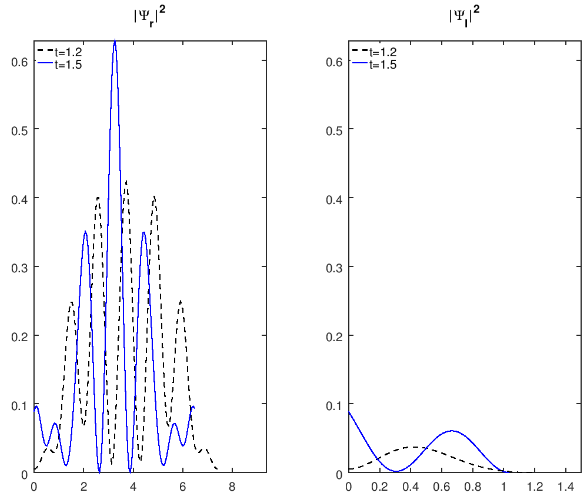

FIG. 6. The wave function at the ring (left) and segment (right) $t = 1.2$, $t = 1.5$ (arbitrary units)

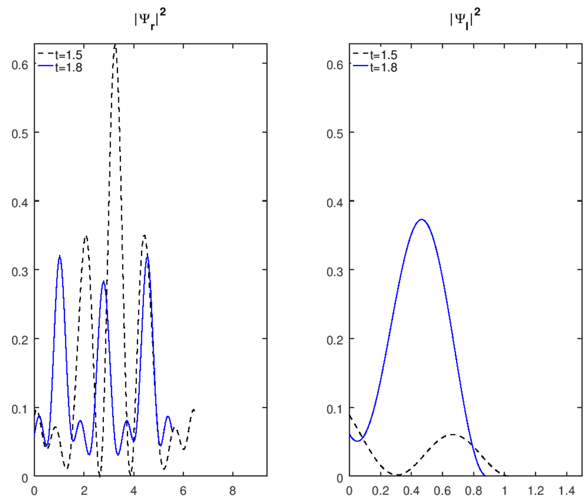

FIG. 7. The wave function at the ring (left) and segment (right) $t = 1.5$, $t = 1.8$ (arbitrary units)

The wave function for the time moment t is obtained by the procedure described in the previous section. The following parameters are chosen: $a = 1$, $b = 1/2$, $\omega = 1$, $r = 1$. Time evolution of the wave packet is shown in Figs. 2–7, corresponding to time values $t = 0$, $t = 1.1$, $t = 1.3$, $t = 1.4$ in initial coordinate system.

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