Time-dependent quantum graph

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In this paper, we study quantum star graphs with time-dependent bond lengths. Quantum dynamics are treated by solving Schrodinger equation with time-dependent boundary conditions given on graphs. The time-dependence of the average kinetic energy is analyzed. The space-time evolution of a Gaussian wave packet is treated for an harmonically breathing star graph.

Keywords: quantum graph,time-dependent boundary conditions,wave packet dynamics.

1. Introduction

Quantum particle dynamics in nanoscale networks and discrete structures is of fundamental and practical importance. Usually, such systems are modeled by so-called quantum graphs. These systems have attracted much attention in physics [1–3] and mathematics [5–7] over the past two decades.

In physics, quantum graphs were introduced as a toy model for studies of quantum chaos by Kottos and Smilansky [1]. However, the concept of studying a system confined to a graph dates back to Pauling [4], who suggested the use of such systems for modeling free electron motion in organic molecules. Over the last two decades, quantum graphs have found numerous applications in modeling different discrete structures and networks in nanoscale and mesoscopic physics (e.g., see reviews [1–3] and references therein).

Mathematical properties of the Schrödinger operators on graphs [5–7] and inverse problems for quantum graphs [8,9], were also the subject of extensive research recently. Also, an experimental realization of quantum graphs is discussed in Ref. [5, 10, 11]. Despite the certain progress made in the study of quantum graphs, some important aspects still remain relatively unexplored. This is especially true for problems of driven graphs, i.e. graphs perturbed by time-dependent external forces. An important example of such a driving force is that caused by driven (moving) boundaries. Treatment of such system requires solving the Schrödinger equation with time-dependent boundary conditions. Earlier, the problem of time-dependent boundary conditions in the Schrödinger equation has attracted much attention in the context of quantum Fermi acceleration [12–14], although different aspects of the problem were treated by many authors [16–27]. Detailed study of the problem can be found in a series of papers by Makowski and co-authors [21–23]. It was pointed out in the above Refs. 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 [21].

In this paper, we treat a similar problem for quantum star graph, i.e. we study the problem of quantum graphs with time-dependent bonds. In particular, we consider

harmonically breathing quantum star graphs, cases of monotonically contracting and expanding graphs. The latter can be solved exactly analytically. Motivation for the study of time-dependent graphs comes from such practically important problems as quantum Fermi acceleration in nanoscale network structures, tunable particle transport in quantum wire networks, molecular wires, different lattices and discrete structures. In particular, sites, vertices, nodes of such discrete structures can fluctuate, which makes them time-dependent. We will study the time-dependence of the average kinetic energy and wave packet dynamics in harmonically breathing graphs.

Graphs are systems consisting of bonds which are connected at the vertices. The bonds are connected according to a rule which is called the topology of a graph. The topology of a graph is given in terms of adjacency matrix [1, 2]:

$$C_{ij} = C_{ji} = \begin{cases} 1, & \text{if } i \text{ and } j \text{ are connected;} \\ 0, & \text{otherwise.} \end{cases} \quad i, j = 1, 2, ..., V. \tag{1}$$

Quantum dynamics of a particle on a graph is described by a one-dimensional Schrödinger equation [1, 2] (in the units $\hbar = 2m = 1$):

$$-i \frac{d^2}{dx^2} \Psi_b(x) = k^2 \Psi_b(x), \quad b = (i, j), \tag{2}$$

where b denotes a bond connecting ith and $j$the vertices, and for each bond b, the component Ψ_b of the total wavefunction Ψ_b is a solution of Eq.(2).

The wavefunction, Ψ_b, satisfies boundary conditions at the vertices, which ensures continuity and current conservation [1]. The general scheme for finding eigenfunctions and eigenvalues for such boundary conditions can be found in Ref. [1]. Different types of boundary conditions for the Schrodinger equation on graphs are discussed in the Refs. [5–7]. In the following, we restrict our consideration to the simplest graph, the so-called star graph. The star graph consists of three or more bonds connected at a single vertex which is called the branching point. Other points are called edge vertices. The eigenvalue problem for a star graph with N bonds is given by the following Schrödinger equation:

$$-\frac{d^2}{dx^2} \phi_j(y) = k^2 \phi_j(y), \quad 0 \leqslant y \leqslant l_j, \ j = 1, ..., N. \tag{3}$$

Here we consider the following boundary conditions [11]:

$$\begin{cases} \phi_1|_{y=0} = \phi_2|_{y=0} = ... = \phi_N|_{y=0}, \\ \phi_1|_{y=l_1} = \phi_2|_{y=l_2} = ... = \phi_N|_{y=l_N} = 0, \\ \sum_{j=1}^{N} \frac{\partial}{\partial y} \phi_j|_{y=0} = 0. \end{cases} \tag{4}$$

The eigenvalues can be found by solving the following equation [11]:

$$\sum_{j=1}^{N} \tan^{-1}(k_n l_j) = 0, \tag{5}$$

where the corresponding eigenfunctions are given as [11]:

$$\phi_j^{(n)} = \frac{B_n}{sin(k_n l_j)} sin(k_n(l_j - y)), \tag{6}$$

where normalization coefficients are given as:

$$B_n = \left[\sum_j (L_j + \sin(2k_n L_j)) \sin^{-2}(k_n L_j)/2 \right]^{-1/2}. \tag{7}$$

2. Time-dependent graph

A time-dependent graph implies that the lengths of the bonds of a graph are time-varying, i.e., when L_j is a function of time. In this case, the particle dynamics in graph are described by the following time-dependent Schrödinger equation:

$$i\frac{\partial}{\partial t}\Psi_j(x,t) = -\frac{\partial^2}{\partial x^2}\Psi_j(x,t), \quad 0 < x < L_j(t), \quad j = 1, ..., N, \tag{8}$$

with N being the number of bonds.

In the following, we will consider the boundary conditions given by:

$$\begin{cases} \Psi_1|_{x=0} = \Psi_2|_{x=0} = ... = \Psi_N|_{x=0}, \\ \Psi_1|_{x=L_1(t)} = \Psi_2|_{x=L_2(t)} = ... = \Psi_N|_{x=L_N(t)} = 0, \\ \sum_{j=1}^{N} \frac{\partial}{\partial x}\Psi_j|_{x=+0} = 0. \end{cases} \tag{9}$$

These boundary conditions imply that only edge vertices of the graph are moving while the center (branching point) is fixed. Furthermore, we assume that $L_j(t)$ is given as $L_j(t) = l_j L(t)$, where $L(t)$ is a continuous function and l_j are positive constants. Then, using the coordinate transformation:

$$y = \frac{x}{L(t)}, \tag{10}$$

Eq.(8) can be rewritten as:

$$i\frac{\partial}{\partial t}\Psi_j(y,t) = -\frac{1}{L^2}\frac{\partial^2}{\partial y^2}\Psi_j(y,t) + i\frac{\dot{L}}{L}y\frac{\partial}{\partial y}\Psi_j(y,t), \quad 0 < y < l_j, \quad j = 1, ..., N. \tag{11}$$

It is clear that the Schrödinger operator in the right hand side of Eq.(11) is not Hermitian due to the presence of a second term. Therefore, using the transformation:

$$\Psi_j(y,t) = \frac{1}{\sqrt{L}}e^{i\frac{L\dot{L}}{4}y^2}\varphi_j(y,t), \tag{12}$$

we can make it Hermitian as:

$$i\frac{\partial}{\partial t}\varphi_j(y,t) = -\frac{1}{L^2}\frac{\partial^2}{\partial y^2}\varphi_j(y,t) + \frac{L\ddot{L}}{4}y^2\varphi_j(y,t), \quad 0 < y < l_j, \quad j = 1, ..., N. \tag{13}$$

We note that the functions $\varphi_j(y,t)$ satisfy the boundary conditions (9) with $y = l_j$ instead of $x = L_j(t)$.

Time and coordinate variables in Eq.(13) can be separated only in the case when $L(t)$ obeys the equation:

$$\frac{L^3\ddot{L}}{4} = -C^2 = const, \tag{14}$$

In this case, using the substitution $\varphi_j(y,t) = \phi_j(y) \exp\left(-ik^2 \int\limits_0^t L^{-2}(s)ds\right)$, we get:

$$\frac{d^2}{dy^2}\phi_j + (k^2 - C^2y^2)\phi_j = 0, \quad y \in (0, l_j). \tag{15}$$

For $C \neq 0$ from Eq.(14), we have:

$$L(t) = \sqrt{\alpha t^2 + \beta t + \gamma}, \quad C^2 = \frac{1}{16}(\beta^2 - 4\alpha\gamma), \tag{16}$$

and

$$L(t) = \sqrt{\beta t + \gamma}, \quad C^2 = \frac{1}{16}\beta^2. \tag{17}$$

In both cases, exact solutions of Eq.(13) can be obtained in terms of confluent hypergeometric functions. In particular, for the case when the time-dependence of $L(t)$ is given by Eq.(17), fundamental solutions of Eq.(13) can be written as:

$$\phi_{j,1} = y \exp\left(\frac{C}{2}y\right) M\left(\frac{3}{4} - \frac{k}{4C}, \frac{3}{2}, -Cy^2\right),$$

and

$$\phi_{j,2} = \exp\left(\frac{C}{2}y\right) M\left(\frac{1}{4} - \frac{k}{4C}, \frac{1}{2}, -Cy^2\right).$$

Therefore, the general solution of Eq.(13) is given as:

$$\phi_j(y) = D_j\phi_{j,1} + G_j\phi_{j,2}, \quad D_j, G_j = const. \tag{18}$$

From the boundary conditions given by Eq.(4), we have:

$$G_j = A, \quad D_j = A \cdot \alpha_j(k), \quad j = 1, 2, 3, ..., N,$$

where A is an arbitrary constant and:

$$\alpha_j(k) = -\frac{M\left(\frac{1}{4} - \frac{k}{4C}, \frac{1}{2}, -Cl_j^2\right)}{l_j M\left(\frac{3}{4} - \frac{k}{4C}, \frac{3}{2}, -Cl_j^2\right)}, \quad j = 1, 2, ..., N.$$

Taking into account the relations:

$$\left.\frac{d\phi_{j,1}(y)}{dy}\right|_{y=0} = 1, \quad \left.\frac{d\phi_{j,2}(y)}{dy}\right|_{y=0} = \frac{C}{2},$$

from Eq.(4), we obtain the following spectral equation for finding the eigenvalues, k_n of Eq.(13):

$$\sum_{j=1}^{N} \frac{1}{l_j} \frac{M\left(\frac{1}{4} - \frac{k}{4C}, \frac{1}{2}, -Cl_j^2\right)}{M\left(\frac{3}{4} - \frac{k}{4C}, \frac{3}{2}, -Cl_j^2\right)} = \frac{CN}{2}. \tag{19}$$

Thus, the eigenfunctions of Eq.(13) can be written as:

$$\phi_j(y, k_n) = A\left[\alpha_j(k_n)\phi_{j,1}(y) + \phi_{j,2}(y)\right], \quad j = 1, 2, ..., N. \tag{20}$$

Furthermore, we provide the solution for Eq.(13) for the simplest case $L(t) = at + b$, which corresponds to $C = 0$ in Eq.(14). In this case, the eigenvalues for Eq.(13), which can be written in terms of the time-dependence of the wall are given as:

$$\phi_j(y, k_n) = \frac{A}{sin(k_n l_j)} sin(k_n(l_j - y)), \quad j = 1, 2, ..., N, \tag{21}$$

where k_n is the nth positive root of the equation:

$$\sum_{j=1}^{N} \tan^{-1}(l_j k) = 0. \tag{22}$$

and $L(t) > 0$, A is the normalization constant.

Now, let us consider the harmonically breathing graph, i.e. the case when the time-dependence of $L(t)$ is given as:

$$L(t) = b + a \cos \omega t,$$

with $\omega = 2\pi T^{-1}$ being oscillation frequency and T is the oscillation period. It is clear that in this case, the time and coordinate variables in Eq.(13) cannot be separated. Expanding $\varphi(y,t)$ in Eq.(13) in terms of the complete set of static graphs solutions gives the wave functions as:

$$\varphi_j(y,t) = \sum_n C_n(t)\phi_j^{(n)}(y), \tag{23}$$

and inserting this expansion into Eq.(13) we have:

$$\dot{C}_m(t) = \sum_n M_{mn}C_n(t),$$

where

$$M_{mn} = -i\frac{k_m^2}{L^2(t)} - i\frac{L\ddot{L}}{4} \sum_j \int_0^{l_j} y^2 \phi_j^{(n)}\phi_j^{(m)}dy.$$

3. Wave packet evolution in harmonically breathing graph

The quantity we are interested in computing is the average kinetic energy, which is defined as:

$$E(t) = \langle \psi|H|\psi\rangle = \sum_{j=1}^N \int_0^{L_j(t)} \left|\frac{\partial \psi_j(x,t)}{\partial x}\right|^2 dx. \tag{24}$$

In Figure 1, the time dependence of the average kinetic energy of the harmonically breathing star graph is presented for different breathing frequency and amplitude values. As can be seen from these plots, $\langle E(t)\rangle$ is almost periodic for $\omega = 0.5$ and $a = 1$, while for $\omega = 10$ and $a = 1$, such periodicity is completely broken and energy increases with time. For $\omega = 10$ and $a = 20$, $\langle E(t)\rangle$ demonstrates "quasiperiodic behavior". The appearance of periodic behavior in $\langle E(t)\rangle$ can be explained by synchronization of the particle motion with the frequency. Over time, the lack of such synchronization causes break in the periodicity of the average energy.

Additionally, we consider wave packet evolution in an harmonically breathing star graph by taking the wave function at $t = 0$ (for the first bond) as the following Gaussian wave packet:

$$\Psi_1(x,0) = \Phi(x) = (2\pi\sigma^2)^{-1/2} \exp\left(-(x-\mu)^2/2\sigma\right), \tag{25}$$

with σ being the width of the packet. For other bonds, the initial wave function is assumed to be zero, i.e. $\Psi_2(x,0) = \Psi_3(x,0) = 0$. Then, for the initial values of the functions $\varphi^{(j)}(y,t)$ in Eq.(23) we have:

$$\varphi_j(y,0) = L(0)e^{-i\frac{L(0)\dot{L}(0)}{4}y^2}\Phi(y).$$

Correspondingly, the expansion coefficients at $t = 0$ can be written as:

$$C_n(0) = \sum_j \int_0^{l_j} \varphi_j(y,0)\phi_j^{(n)*}(y).$$

In calculating the wave packet evolution, we choose the initial condition as the Gaussian wave packet being on the first bond only, while for the other two bonds, the wave functions at $t = 0$ are taken as zero. In Figure 2, the time evolution of the wave packet is plotted for
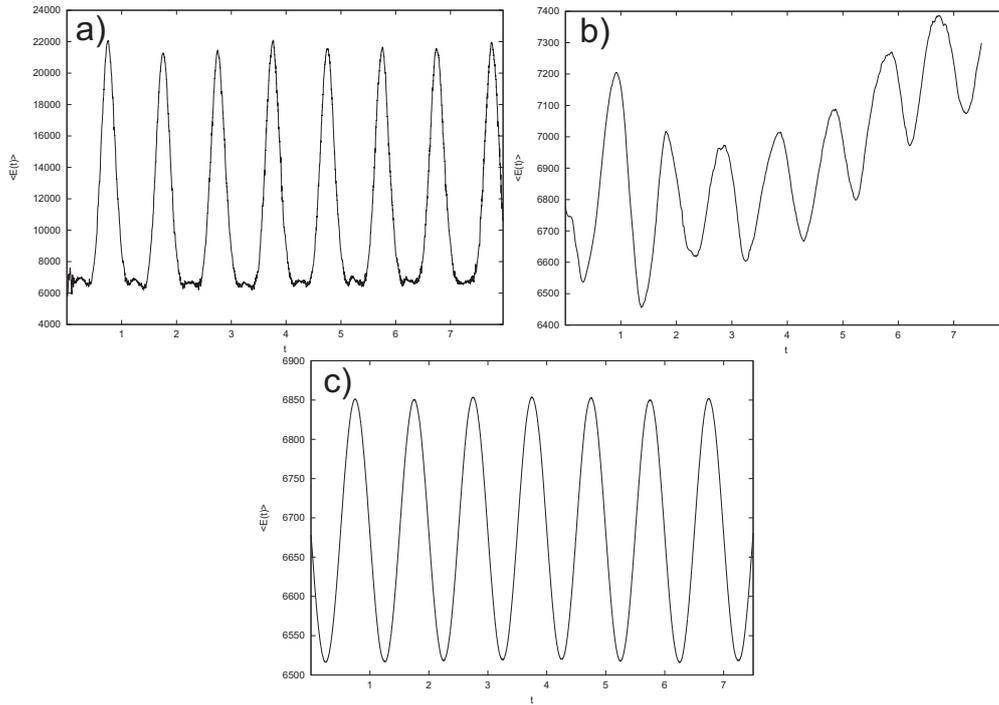
FIG. 1. Time-dependence of the average kinetic energy for an harmonically oscillating primary star graph. Time is presented in the units of the oscillation period $T = 2\pi/\omega$
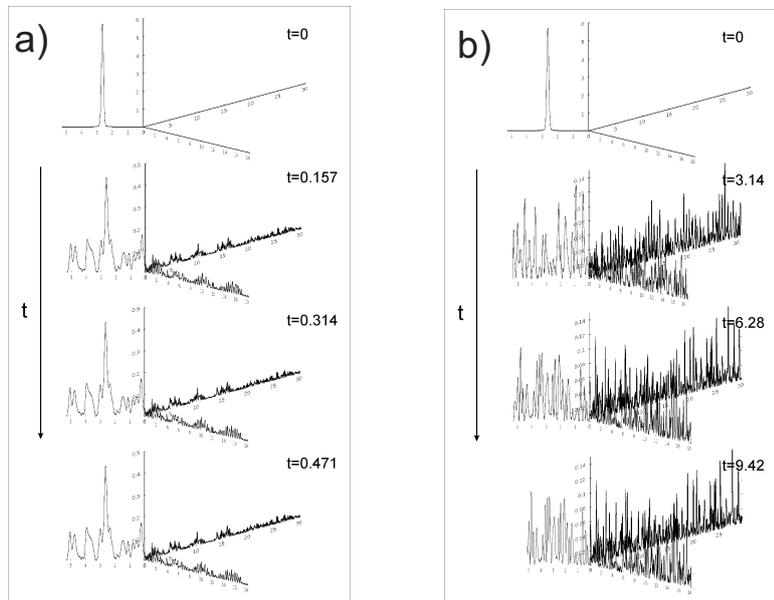
FIG. 2. Time evolution of the Gaussian wave packet given by Eq.(25) for the parameters: a) Wave packet evolution in static star graph b) $\omega = 0.5$, $a = 1$;.
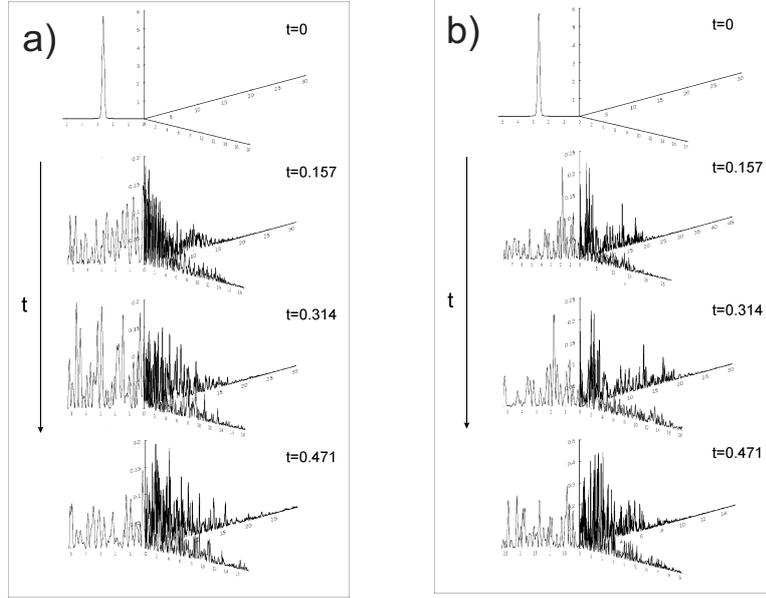
FIG. 3. Time evolution of the Gaussian wave packet given by Eq.(25) for the parameters: a) $\omega = 10$, $a = 20$; b) $\omega = 10$, $a = 1$;.

an harmonically breathing primary star graph whose bonds oscillate according to the law $L(t) = 40 + a\cos\omega t$. The oscillation parameters (frequency and amplitude) are chosen as follows: a) $\omega = 10$, $a = 20$; b) $\omega = 10$, $a = 1$; c) $\omega = 0.5$, $a = 1$. Figure 2a presents wave packet evolution in a static(time-independent) star graph. At $t = 0$, a Gaussian packet of width σ and velocity v_0 is assumed being in the first bond. As can be seen from these plots, for higher frequencies, dispersion of the packet and its transition to other bonds occurs more quickly compared to that of smaller frequencies. Again, an important role is played here by the possible synchronization between the bond edge and wave packet motions. The existence or absence of such synchronization defines how the collision of the packet with the bond edges will occur and how extensively it gains or loses its energy. Therefore, a more detailed treatment of the wave packet dynamics in harmonically breathing graphs should be based on the analysis of the role of synchronization and its criteria. Figure 4 presents time evolution of the probability densities corresponding to plots in Figure 2 and Figure 3. The parameters of the wave packet and oscillation parameters are the same as those in Figure 2 and Figure 3.

4.   Conclusions

In this paper, we have treated a time-dependent quantum network by considering monotonically expanding and harmonically breathing quantum star graphs. Edge boundaries were considered to be time-dependent, while the branching point was assumed to be fixed. The time-dependence of the average kinetic energy and space-time evolution of the Gaussian wave packet were studied by solving the Schrodinger equation with time-dependent boundary conditions. It was found that for certain frequencies, energy is a periodic function of time, while for others, it can be a non-monotonically growing function of time. Such a feature can be caused by possible synchronization of the particles' motion and the motions of the moving edges of graph bonds. A similar feature can also be seen in the analysis of wave packet evolution. The above study can be useful for the treatment of particle transport
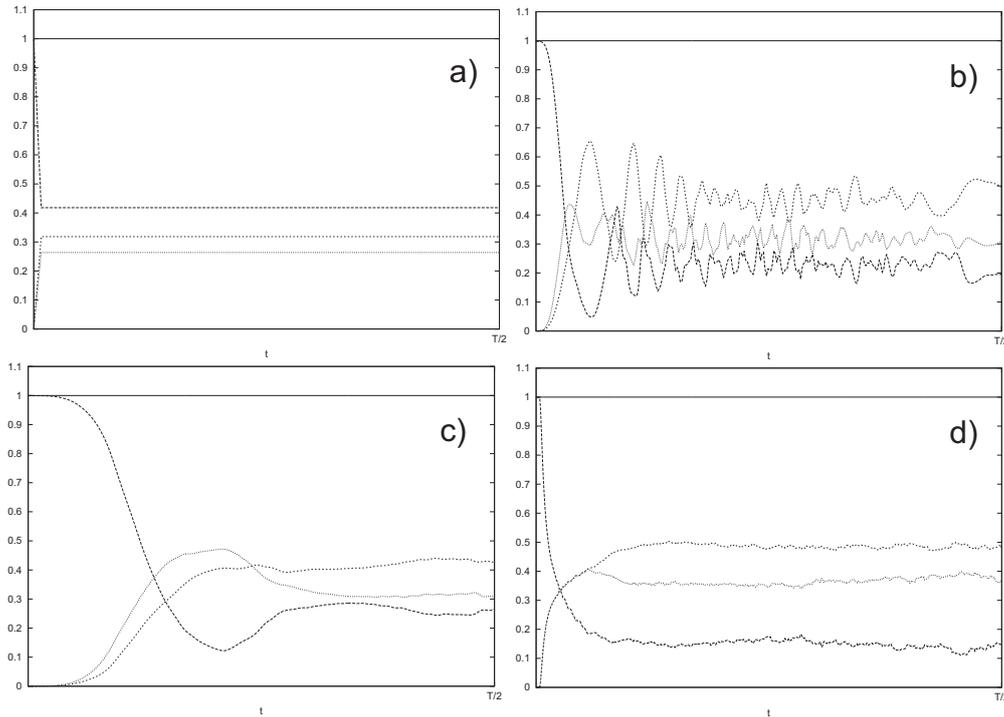
FIG. 4. Time evolution of the probability density: a) for static graph; b) time-dependent graph with $\omega = 10$ and $a = 20$; c) time-dependent graph with $\omega = 10$, and $a = 1$; d) time-dependent graph with $\omega = 0.5$, and $a = 1$.

in different discrete structures, such as molecular and quantum wire networks, networks of carbon nanotubes, crystal lattices, and others nanoscale systems that can be modeled by quantum graphs.

Acknowledgements

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