NANOSYSTEMS:
PHYSICS, CHEMISTRY, MATHEMATICS

Blinova I.V., et al. *Nanosystems: Phys. Chem. Math.*, 2022, **13** (3), 245–249.
http://nanojournal.ifmo.ru
DOI 10.17586/2220-8054-2022-13-3-245-249

Original article

Spectral gaps for star-like quantum graph and for two coupled rings

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ABSTRACT The spectral problems for two types of quantum graphs are considered. We deal with star-like graph and a graph consisting of two rings connected through a segment. The spectral gap, i.e. the difference between the second and the first eigenvalues of the free Schrödinger operator, is studied. The dependence of the gap on the geometric parameters of the graph is investigated. Particularly, it is shown that the maximal gap is observed for the symmetric quantum graph.

KEYWORDS spectral gap, quantum graph, Schrödinger operator, discrete spectrum.

FOR CITATION Blinova I.V., Popov A.I., Bosova A.A. Spectral gaps for star-like quantum graph and for two coupled rings. *Nanosystems: Phys. Chem. Math.*, 2022, **13** (3), 245–249.

1. Introduction

The most adequate models of quantum system (particularly, for nanosystems) is ab initio methods. But using of such approaches is not simple due to great computational complexity. The situation changes if a particle under consideration cannot leave a submanifold of less dimension [1–4]. It allows one to reduce the problem to a task on this manifold or several manifolds [5]. Correspondingly, an important point is a way of gluing of solutions on different manifolds. It can be made in the framework of the theory of self-adjoint extensions of symmetric operators [6–11]. The simplest model of such type is quantum graph. Rigorous mathematical theory of quantum graphs was constructed last decades [12–14]. Hybrid manifolds were studied in less extent [3, 15, 16]. It was shown that such models are effective for description of spectral properties of operators. Some approaches were developed in this field (Krein's formula approach, boundary triplets method, spaces of boundary values).

In our paper, the spectral gap for a few simple quantum graphs is determined and a relation to graph surgery is discussed. One can mention recent results concerning to quantum graph problems related to the present paper [17–21].

The quantum graph is a set of vertices and edges. At each edge e_i, we consider the free Schrödinger operator

$$H_i = \frac{d^2}{dx^2}$$

with the domain $W_2^2(e_i)$ acting in the space $L_2(e_i)$. Here $W_2^2(e_i)$ is the Sobolev space. The state space for the whole graph is $\sum_i \oplus L_2(e_i)$. To determine the Hamiltonian for the graph, we consider the operator H_i at each edge and impose a coupling condition at the graph vertices. We choose the Kirchhoff condition. It means that a function from the operator domain should be continuous on the graph, particularly, at vertices, i.e. it should have the same boundary value at each edge e_{ji}, e_{pi} adjacent to the vertex v_i:

$$\psi_j(v_i) = \psi_p(v_i). \tag{1}$$

The second condition at the vertex v_i is vanishing of the algebraic sum over all adjacent vertices of derivatives:

$$\sum_{e_{ji}} (-1)^{\nu_{ji}} \psi_j(v_i) = 0, \tag{2}$$

where $\nu_{ji} = 1$ if the edge e_{ji} is outgoing from the vertex v_i and $\nu_{ji} = -1$ if the edge e_{ji} is incoming to the vertex v_i. As for the boundary vertices of the quantum graph, we assume the Dirichlet boundary condition here

$$\psi_j(v_i) = 0. \tag{3}$$

We consider quantum graphs with finite number of edges of finite lengths, correspondingly, the Hamiltonian has purely discrete spectrum. To solve the spectral problem, it is necessary to solve the equation

$$-\psi_i''(x) = \lambda \psi_i(x)$$

at each edge e_i and to satisfy the boundary conditions at all vertices.

2. Spectral gap

2.1. Star-like graph

Consider a star-type graph with 5 vertices and 4 edges and study the dependence of the spectral gap on the ratio of edge lengths.

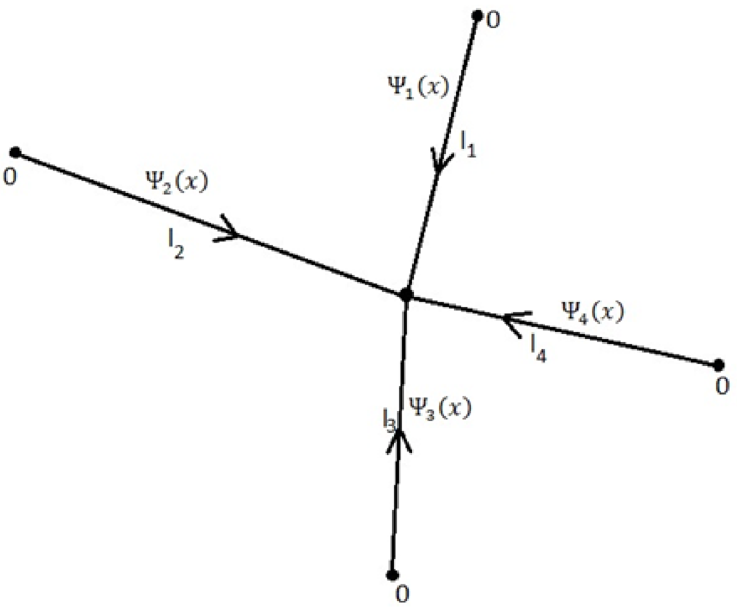

FIG. 1. Graph with 5 vertices and 4 edges

On each edge of the graph, the solution has a form $\psi = a\cos kx + b\sin kx$. The coefficients are determined from the conditions at the vertices. On the edges $e_1,\ e_2,\ e_3,\ e_4$ of lengths $l_1,\ l_2,\ l_3,\ l_4$, correspondingly, functions $\psi_1(x),\ \dots,\psi_4(x)$ are given by the following expressions

$$\begin{cases} \psi_1(x) = A\cos kx + B\sin kx, \\ \psi_2(x) = C\cos kx + D\sin kx, \\ \psi_3(x) = E\cos kx + F\sin kx, \\ \psi_4(x) = H\cos kx + G\sin kx. \end{cases}$$

Let us write down the system of coupling conditions at the vertices. Boundary conditions (1), (2), (3)) lead to a system of homogeneous equations for the coefficients. The condition for the system to have a nontrivial solution is that its determinant is equal to zero. This gives us the spectral equation:

$$\sin kl_1 \sin kl_2 \sin kl_3 \cos kl_4 + \sin kl_1 \sin kl_4 \sin kl_3 \cos kl_2 + \sin kl_2 \sin kl_4 \sin kl_3 \cos kl_1 + \sin kl_1 \sin kl_2 \sin kl_4 \cos kl_3 = 0. \quad (4)$$

Eigenvalues $\lambda_i = k_i^2$, where k_i is the $i-$th root of the spectral equation (4), are positive and they are ordered increasingly. The spectral gap is the difference between the second and first eigenvalues. Let's see how the spectral gap changes if one varies the lengths of edges. To ensure the comparability of the gaps,, we preserve the total length of the graph L unchanged for all such transformations. Let us take the unit total length for simplicity: $L = 1$. Consider the following variation of lengths:

$$l_1 = L + \delta, \quad l_2 = L - \frac{\delta}{3}, \quad l_3 = L - \frac{\delta}{3}, \quad l_4 = L - \frac{\delta}{3}.$$

Figure 2. shows the dependence of the spectral gap on the value of δ. One can see that the maximal value of the spectral gap is observed for the symmetric case when all edges are equal ($\delta = 0$). The graph in Fig. 2 is not even in respect to δ because the perturbation is not symmetric: the length of one edge increases and the lengths of three edges decrease. In case of two increasing and two decreasing lengths, the graph is even, naturally.

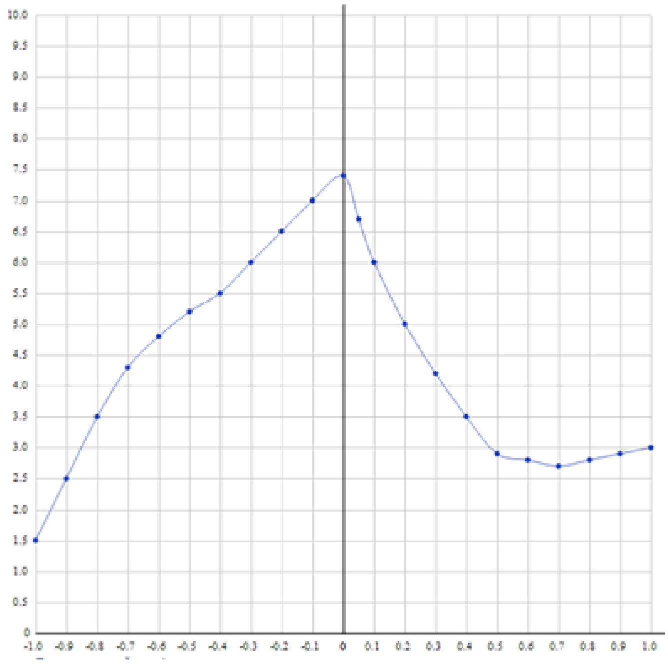

FIG. 2. Dependence of the spectral gap on the value of δ; dimensionless units

2.2. Two coupled loops

Consider a graph with two loops coupled by one edge. It is shown in Fig. 3. Parameter x at the rings is the length of the arc starting from the vertex. It should be noted that in the considered case, the curvature of the edge does not play a role.

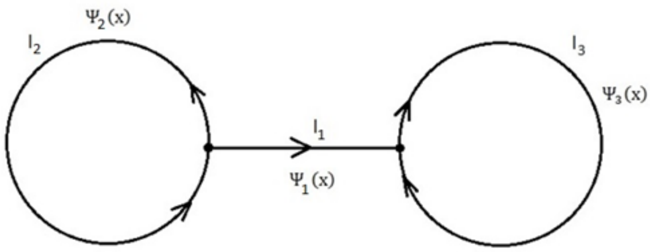

FIG. 3. Two coupled loops

On each edge of the graph, the solution has the following form $\psi(x) = a\cos kx + b\sin kx$. The coefficients are determined from the conditions at the vertices. In this case, the spectral equation has the form:

$$-\sin\left(\frac{kl_1}{2}\right)\sin\left(\frac{kl_3}{2}\right)\times \left(2\sin(kl_2)\left(5\cos\left(\frac{1}{2}k(l_1+l_3)\right)-3\cos\left(\frac{1}{2}k(l_1-l_3)\right)\right)+8\sin\left(\frac{1}{2}k(l_1+l_3)\right)\cos(kl_2)\right)=0.$$

We vary the lengths of the edges preserving the total length of the graph unchanged, i. e. $L = 1$. Consider the following symmetrical and asymmetrical length variations:

$$\begin{cases} 1)\ l_1 = L+\delta,\ \ l_2 = L-\dfrac{\delta}{2},\ \ l_3 = L-\dfrac{\delta}{2}. \\ 2)\ l_1 = L+\delta,\ \ l_2 = L-\dfrac{5}{6}\delta,\ \ l_3 = L-\dfrac{\delta}{6}. \\ 3)\ l_1 = L-\dfrac{\delta}{4},\ \ l_2 = L-\dfrac{3}{4}\delta,\ \ l_3 = L+\delta. \end{cases} \tag{5}$$

Figure 4 shows plots of the spectral gap versus δ for these three cases. One can see that curve 1 corresponding to the symmetric perturbation lies above curves 2,3. It is interesting that there are also such values of the perturbation which correspond to minima of the graph of this dependence.

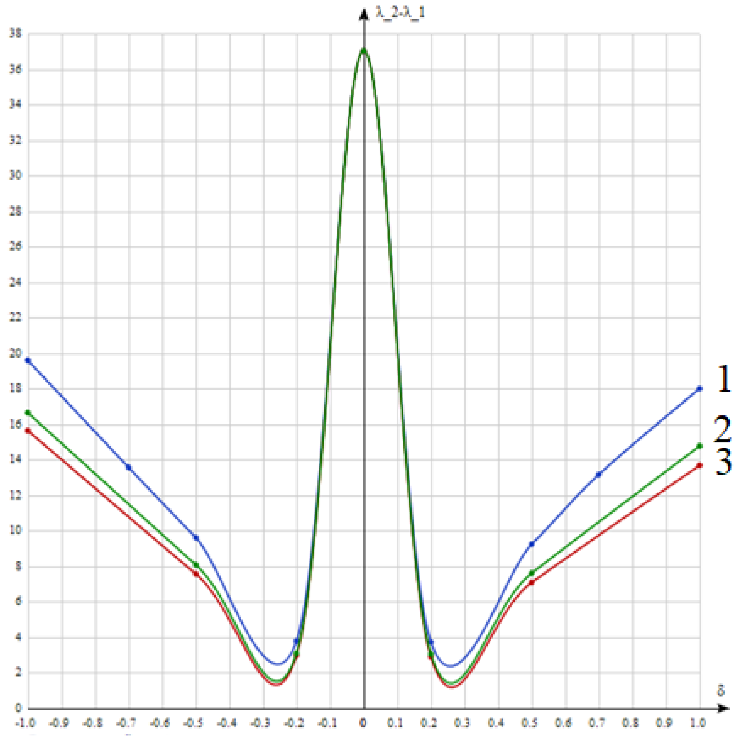

FIG. 4. Plots of the spectral gap versus δ; curves 1, 2, 3 correspond to cases in (5); dimensionless units.

Thus, consideration of these two types of quantum graphs leads to the conclusion that the value of the spectral gap depends on the symmetry of the graph and the ratio of the lengths of the edges. The largest gap is obtained in a symmetrical situation. Any breaking of symmetry leads to the decreasing of the spectral gap.

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Submitted 05 April 2022; revised 01 June 2022; accepted 14 June 2022

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Conflict of interest: the authors declare no conflict of interest.