Discrete spectrum for quantum graph with local disturbance of the periodicity

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Abstract. The problem of discrete spectrum for quantum graph with local disturbance of the periodicity is described. The Hamiltonian is determined as 1D Schrödinger operator on each edge and some boundary conditions at each vertex. The spectral analysis of the quantum graph having the form of branching strips with hexagonal (honeycomb) structure is considered in more details.

1. Introduction
Theoretical investigation of nanostructures, especially, of carbon nanostructures, attracts great attention due to their unusual properties \cite{1, 2, 3} and the existing or expected applications. The studying of complex nanostructures on the background of the mathematical theory of differential operators on graphs — a rapidly developing field of modern mathematical physics, whose significance is related with possible applications to solid state physics and nanoelectronics as a whole \cite{4}.

A start of intensive studying of differential operators on metric graphs was in 80th (see works of N.I. Gerasimenko and B.S. Pavlov \cite{5}, P. Exner and P. Šeba \cite{6}). One can mention that the quantum graph problem is related with the corresponding discrete operator. In recent years the model of quantum graphs was widely used and allowed one to get many interesting results. An overview of new results and open problems can be found in the book \cite{2}.

Quantum graph is determined by a second order self-adjoint differential operator defined at the edges of the metric graph, viewed as intervals, and certain boundary conditions at the vertices. The differential operators describe the movement of a quantum particle along the edges. The choice of the operator is related with the physical motivation. It can be 1D free Schrödinger (for non-relativistic particle) or Dirac (e.g., for an electron in graphene) operator or the Hamiltonian with external electric or magnetic field. The boundary conditions specify the transition probabilities across the vertices. Quantum graphs are used as simplified models in many situations involving wave propagation. One-dimensional type of the structure allows one to obtain many results in an explicit form. On the other hand, the graph structure can be sufficiently complicated, and it allows one to describe quite complex and useful models. The description of the operator spectrum is a natural problem for quantum graphs, because it is related with interesting physical phenomena.
2. Local perturbations and discrete spectrum

Purely periodic quantum graphs have no discrete spectrum (it can have only continuous spectrum or eigenvalues of infinite multiplicity) but any local perturbation create a possibility of its appearance [7, 8, 9]. The information about the bound states is very essential for description of physical properties of nanosystems. There is a natural question: "Under what condition does the disturbance lead to a bound state appearance?". At present, one has no general answer. However, a collection of results in this direction has been obtained.

At first, let us consider the Schrödinger operator on a line with δ–potentials at the points \( nT_1, n \geq 0 \); \( nT_2, n < 0 \). It can be considered as two semi-infinite quantum graphs with different edges lengths coupled at 0. In principle, an eigenvalue can appear, but Albeverio with co-authors [10] showed that the discrete spectrum is empty. The analogous problems for the Schrödinger operator on a line with locally perturbed smooth periodic potential were studied by many authors (see, e.g., [11, 12, 13, 14, 15, 16]). There are also a number of works dealing with the corresponding 2D or 3D nanosystems. Considerable attention of physicists is attracted to the construction of nanostructures based on nanotubes [17]. An interesting example of such nanostructure was recently created experimentally [18, 19]. It is a junction of two nanotubes of zigzag and armchair types (see Fig. 1).

\[ \text{Figure 1. Armchair-zigzag junction} \]

In this system the crystal structure is broken at the interface. This is a reason for appearance of localized states [20]. Different mathematical models were suggested to describe the effect [21, 22, 23, 24]. Particularly, the authors of [23, 24] deal with quantum graph model. They obtained necessary and sufficient conditions ensuring the existence of bound states localized near the interface.

Another interesting locally perturbed periodic physical nanosystems are nanostructures of chain type. There are works describing these systems in the framework of the quantum graph model. The first mathematical result in this direction is obtained in the work [7]. The authors solve the one-dimensional spectral problem on an infinite quantum graph consisting of identical rings connected at the touching points by δ-couplings with a parameter \( \alpha \in \mathbb{R} \). The "bending" deformation of the chain (i.e. variation of the position of one touching point at one ring) is considered. Using the method of the transfer-matrices, the authors show that this local perturbation leads to an appearance of eigenvalues in the open spectral gaps. The eigenvalues positions depend on the bending angle. The continuous spectrum does not depend, naturally,
on the bending angle. It is determined by the transfer-matrix only, i.e. it coincides with the continuous spectrum for the straight chain. The analogous problem for Y-branched chain was considered in [9]. It is interesting to note that in the both cases the discrete spectrum is empty if there are no $\delta$-potentials at the touching points, i.e. if one has the Kirchhoff condition at the graph vertices. At present, it is not known how general is this statement, e.g., does it depend on the graph structure?

To evaluate this hypothesis, we consider a quantum graph $\Gamma$, consisting of three symmetrically coupled semi-infinite strips, shown in Figure 2. It can be a model of a nanosystem with honeycomb lattice, e.g., carbon nanoribbon. Although each strip is invariant in respect to a semi-group of translations, the system is not periodic, and the discrete spectrum of the Hamiltonian can exist. The spectral analysis of the system is made in [25]. Let us describe it in more details. Let $\mathcal{E}$, $\mathcal{V}$ be, correspondingly, the sets of the graph edges and vertices.

We consider free Schrödinger operator on each edge of the graph $\Gamma$

$$H = -\frac{d^2}{dx^2}$$

and $\delta$-type conditions at the vertices (i.e. the continuity of functions and a "jump" of its derivatives). Correspondingly, the domain of the operator (1) is as follows

$$\text{dom } H = \left\{ f \in C \left( \Gamma \cap H^2 \left( \Gamma - \mathcal{V} \right) \right) \sum_{e \in \mathcal{E}_v} \frac{df}{dx_e} (v) = \alpha f (v) \right\} .$$

Here $H^2$ is the Sobolev space $W^2_2$, $\alpha$ is some fixed number, $\mathcal{E}_v := \{ e \in \mathcal{E} | v \in e \}$ is the set of edges adjacent to the vertex $v$. The sum is taken over all edges $e$ incident to the vertex $v$ and the derivatives are taken along $e$ in the directions away from the vertex $v$ (outgoing direction). One can see that the operator is self-adjoint. This type of the operator is often used in the quantum graph theory (see, e.g., papers [7, 26]). The structure of the spectrum is described in the following theorem (it is schematically shown in Fig. 3, 4).

**Main theorem.** *The structure of the spectrum of the Hamiltonian $H$ for the graph is as follows.*
a) Positive half-axis.

The continuous spectrum has band structure. A point \( E = k^2 \) belongs to the continuous spectrum if

\[
\begin{cases}
|b^+| \leq 2, \\
|b^-| \leq 2,
\end{cases}
\]

\[ b^\pm = 1 \mp 2 \cos kT + 3 \cos 2kT + \frac{\alpha}{k} \sin 2kT. \]

Here \( T \) is the edge length.

There are points of the discrete spectrum in the gaps if

\[ |\alpha| T > \alpha_m T = 2\sqrt{2\sqrt{3}-3} \arccot\sqrt{2\sqrt{3}-3}. \]

b) Negative half-axis.

There is no spectrum on the negative half-axis for \( \alpha \geq 0 \). For \( \alpha < 0 \) the lower bound of the continuous spectrum is \( E_{\text{thr}} = -\chi_0^2 \), where \( \chi_0, \chi_0 > 0 \), is the root of the equation

\[ \cosh \chi T (-1 + 3 \cosh \chi T + \frac{\alpha}{\chi} \sinh \chi T) = 2. \]

There is no discrete spectrum below the threshold \( E_{\text{thr}} \) if \( \alpha_c \leq \alpha < 0 \). There is at least one eigenvalue below the threshold \( E_{\text{thr}} \) if \( \alpha < \alpha_c \). Here

\[ \alpha_c = -T^{-1} \sqrt{3 + 2\sqrt{3}} \ln(1 + \sqrt{3} + \sqrt{3 + 2\sqrt{3}}). \]

One can see that in this case one has a situation analogous to that for more simple graphs of chain type: empty discrete spectrum if there are no \( \delta \)–potentials at the graph vertices.

3. Discussion

Chain type nanostructures are widely used for constructing of elements of nano devices. The availability of the quantum graph model in our case is related with the fact that only electrons having energies, close to the Fermi energy, are involved in the electron transport. It allows one to reduce 3D Schrödinger equation with chain of short-range potentials to 1D one, i.e. to the quantum graph (see, e.g., [27]). Transport properties of the system play a crucial role for nano device creation. In its turn, it strongly depends on the Hamiltonian spectrum. Bound states has an essential effect on electron transport, especially in chain-type nanostructures.

It can be shown by the following qualitative explanation. The density of electrons in a solid (semiconductor) is about \( 10^{19} \text{cm}^{-3} \), thus the distance between them is about \( 10^{-6} \text{cm}^{-1} \) which is typically at least two orders of magnitude larger than the minimal period in the solid. It shows that one-electron approximation is appropriate in many cases. Nevertheless, the interaction between electrons cannot be neglected since various collective effects for the whole system of electrons in the solid are caused by the long-range Coulomb interaction. A practical understanding of the multi-particle aspect on a quantum network might follow the ideology of coupled clusters theory, see for instance [28] and references therein. In our case of branched strips, the effect of the bound state is essentially greater. This state is localized in a neighborhood of the junction. If this energy level is occupied by an electron, then due to Coulomb repulsion, it has great influence on electrons travelling through the junction. The main result of the present paper describes the condition for the bound state appearance which is important for nanoelectronic devices (to ensure a proper transport properties).

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**Figure 3.** Spectrum for negative alpha

**Figure 4.** Spectrum for positive alpha

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