

On the Spectrum Discreteness for the Magnetic Schrödinger Operator on Quantum Graphs

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ABSTRACT. The aim of this work is to study the discreteness of the spectrum of the Schrödinger operator on infinite quantum graphs in a magnetic field. The problem was solved on a set of quantum graphs of a special kind.

1. Introduction

For the operator describing a physical system, it is an ongoing problem to describe which properties the system characterise when the spectrum of the operator is discrete. This problem has been solved in various special cases. For example, Molchanov proposed in [12] a criterion for a potential to provide the discreteness of the Hamiltonian spectrum in the 1-dimensional case. Necessary and sufficient conditions for a self-adjoint operator on a line related to a general second-order expression to have discrete spectrum are presented in the article [13]. The discreteness of the spectrum of the non-magnetic Schrödinger operator has been studied, for example, in [1, 2, 11, 16]. In the case of a magnetic field, one works in the space of complex functions, which complicates the task. Studies of the magnetic Schrödinger operator were carried out in [3, 6, 7, 10, 14], but no rigorous criteria have been proved for the discreteness of the spectrum of the Schrödinger operator on quantum graphs in a magnetic field. The mathematical modeling of the physical system in this article is based on the theory of quantum graphs. A rigorous proof of the correctness of their use was offered in [15], and the mathematical theory of quantum graphs was treated in [4, 9].

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2. Preliminary

In this article, we confine our attention to some specific quantum graphs only. The class of these graphs is described below.

Definition 2.1. A quantum graph belongs to the class G if it is a connected graph and the following conditions are satisfied:

- (1) any two vertices are connected by no more than a finite set of edges,
- (2) the length of the edges of the graph is bounded below by a positive constant,
- (3) for any fixed vertex v and for any marked edges (the sum of the lengths of all marked edges is equal to infinity) there is a path p satisfying the following properties:
 - (i) p starts at vertex v ;
 - (ii) p is isomorphic to the half-line;
 - (iii) p contains marked edges (not necessarily all), the sum of their lengths is equal to infinity.

Unfortunately, this definition is not illustrative. Two examples of quantum graphs belonging to the class G are: an infinite flat rectangular lattice, and an infinite lattice built on a parallelepiped. It is also worth noting that if some quantum graph G_0 belongs to the class G , then any connected subgraph of the quantum graph G_0 belongs to the class G . We define the magnetic Schrödinger operator H on graphs from the class G in a conventional way (see, e.g., [5, 8]).

Definition 2.2. The domain of the Schrödinger operator on a curve in \mathbb{R}^3 in an electromagnetic field is as follows:

$$\begin{aligned} \text{dom}H &= \{u \in C(G) \cap H^2(G \setminus V(G)); \\ &\sum_{e \in E_v} \partial_{x_e} u(v) = \beta_v u(v), v \in V(G); u(v) = 0, v \in \partial G\}. \end{aligned}$$

The operator acts on each edge of the quantum graph as follows (in dimensionless units):

$$(2.1) \quad Hf(t) = -\left(\frac{\partial}{\partial t} - ia(t)\right)^2 f(t) + q(t)f(t),$$

where $C(G)$ is the space of continuous functions on G , $V(G)$ is the set of vertices G , H^2 is the Sobolev space W_2^2 , E_v is the set of edges containing the vertex v , $\partial_{x_e} u(v)$ is the magnetic derivative of the function for the vertex v lying on the edge e coming out of the vertex v , $\beta_v > 0$ is a real positive number, $\vec{A} : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is the vector potential of the magnetic field, $q(t) : \mathbb{R}^3 \rightarrow \mathbb{R}$ is the scalar potential of the electric field, $a(t) = \frac{dr}{dt}(t) \cdot \vec{A}(r(t))$ is an auxiliary function, $r(t)$ is the

natural parameterization of the curve that is the edge of the quantum graph, and dimensionless parameters are selected as follows: $e = 1, h = 2\pi, m = \frac{1}{2}$.

Note that the variable t is exclusively a parametrization variable and does not carry any physical meaning.

3. Result

We deal with the spectral problem

$$(3.1) \quad Hf = \lambda f.$$

The main result of this article is the following theorem.

Theorem 3.1. *Consider a quantum graph that belongs to the class G . Assume that the function $q(t)$ (see 2.1), which characterizes the scalar potential of the electric field is bounded below and has the following property*

$$(3.2) \quad \lim_{b \rightarrow \infty} \inf_{L_a, \text{dist}(a, v_0) > b} \int_{L_a} q(\tau) d\tau = \infty$$

for any $\omega > 0$ and a fixed vertex v_0 , where L_a belongs to the set of all disjoint paths on the quantum graph under consideration whose length is ω , and a is the starting point of the path L_a (a is the closest to v_0 endpoint of L_a).

For any fixed λ there exist values for the boundary conditions β_v such that any solution of the spectral problem of the operator H on the quantum graph under consideration has a finite number of roots located on this quantum graph.

Note that from the assumption of the theorem it is known that function $q(t)$ is bounded below, which means that there exists some constant c such that $q(t) \geq c$ for any $t \in (0, \infty)$. Suppose that c is not equal to 0, then we make the following change of variables: $\tilde{q}(t) = q(t) - c, \tilde{\lambda} = \lambda + c$. Then, the obtained problem is equivalent to the problem formulated in the hypothesis of the theorem and $q(t) \geq 0$. Thus, we assume in what follows that $q(t) \geq 0$. We carry out the following change of variables for each edge of the quantum graph parameterized by the segment $[0; t_k]$,

$$(3.3) \quad f_k(t) = y_k(t) e^{i \int_0^{t_k} a_k(\tau) d\tau},$$

where the function $a_k(\tau)$ is the restriction of the function $a(\tau)$ to the edge under consideration. Note that the roots of the function $f_k(t)$ coincide with the roots of the function $y_k(t)$; therefore, in the proof of the theorem, we will study the roots of the function $y(t)$, which is the union of the functions $y_k(t)$. Let us prove the theorem by contradiction. Fix a positive λ . Suppose that there is a complex solution to the equation that has an infinite number of roots belonging to the interval $(0, \infty)$. Then from the condition that the quantum graph under consideration belongs to the class

G , it follows that there exists a path L_{v_0} starting at the vertex v_0 , isomorphic to the half-line on which there is an infinite number of roots of the complex function $y(t)$. We denote them as follows: $\alpha_1 < \alpha_2 < \dots < \alpha_n < \dots$. We may assume there is such a chain of roots or there would be a segment with an infinite number of roots on it. This would mean that there is a root condensation point, hence, this solution is identically zero. However, we are looking only for non-trivial solutions. Take some $\omega > 0$, for which it is true that $\omega < (\lambda_0 + 1)^{-1}$. Take b such that for some fixed vertex v_0 the following is true:

$$(3.4) \quad \int_{L_a} q(\tau) d\tau > \omega \cdot (\lambda_0 + 1),$$

where $dist(a, v_0) > b$, which is possible by virtue of the condition (3.2). Let us take n such that $\alpha_n > b$ and m such that $dist(\alpha_m, \alpha_n) > \omega$. Note that in the future we can assume that $\alpha_m - \alpha_n = P\omega$, where P is an integer. We study the original equation for a fixed λ_0 :

$$(3.5) \quad y''(t) = (q(t) - \lambda_0)y(t).$$

We make the following conversion:

$$(3.6) \quad y''(t)\bar{y}(t) = (q(t) - \lambda_0)y(t)\bar{y}(t),$$

where $\bar{y}(t)$ is the adjoint function of the function $y(t)$. We integrate the equation (3.6) from α_n to α_m . We integrate by parts the left hand side of the equation:

$$(3.7) \quad \int_{\alpha_n}^{\alpha_m} y''(t)\bar{y}(t)dt = \sum_{k=1}^s y'_k(v_k)\bar{y}_k(v_k) - \sum_{k=1}^s y'_{k+1}(v_k)\bar{y}_{k+1}(v_k) - \int_{\alpha_n}^{\alpha_m} |y'(t)|^2 dt,$$

where the path between the roots α_n and α_m contains s vertices v_k and $y_k(t)$ is the restriction of the function $y(t)$ to the k -th edge, counting from the point α_n . As for the right side of the equation (3.6), we obtain the following:

$$(3.8) \quad \int_{\alpha_n}^{\alpha_m} (q(t) - \lambda_0)y(t)\bar{y}(t)dt = \int_{\alpha_n}^{\alpha_m} q(t)|y(t)|^2 dt - \lambda_0 \int_{\alpha_n}^{\alpha_m} |y(t)|^2 dt.$$

We carry out the following transformation:

$$(3.9) \quad \int_{\alpha_n}^{\alpha_m} q(t)|y(t)|^2 dt = \sum_{k=1}^P \int_{L_{ak}} q(t)|y(t)|^2 dt,$$

where $L = \cup_k L_{ak}$ is the path connecting the points α_n and α_m , and $|L_{ak}| = \omega$. Using the mean value theorem, we obtain the following inequality:

$$(3.10) \quad \int_{L_{ak}} q(t)|y(t)|^2 dt > (\lambda_0 + 1)|y(\xi_k)|^2 \omega,$$

where $\xi_k \in L_{ak}$. Thus, we can obtain from (3.9), (3.10) the following inequality:

$$\begin{aligned} & \int_{\alpha_n}^{\alpha_m} q(t)|y(t)|^2 dt > (\lambda_0 + 1)\omega \sum_{k=1}^P |y(\xi_k)|^2 \\ & = (\lambda_0 + 1) \cdot \left(\int_{\alpha_n}^{\alpha_m} |y(t)|^2 dt - \sum_{k=1}^P \int_{L_{ak}} (|y(t)|^2 - |y(\xi_k)|^2) dt \right). \end{aligned}$$

After some transformations, the following inequalities can be obtained:

$$\begin{aligned} & \sum_{k=1}^s y'_k(v_k)\bar{y}_k(v_k) - \sum_{k=1}^s y'_{k+1}(v_k)\bar{y}_{k+1}(v_k) - \int_{\alpha_n}^{\alpha_m} |y'(t)|^2 dt \\ & > (\lambda_0 + 1) \int_{\alpha_n}^{\alpha_m} |y(t)|^2 dt - (\lambda_0 + 1)\omega \int_{\alpha_n}^{\alpha_m} |y(t)|^2 dt \\ & \quad - (\lambda_0 + 1)\omega \int_{\alpha_n}^{\alpha_m} |y'(t)|^2 dt - \lambda_0 \int_{\alpha_n}^{\alpha_m} |y(t)|^2 dt \\ & = (\lambda_0 + 1 - (\lambda_0 + 1)\omega - \lambda_0) \int_{\alpha_n}^{\alpha_m} |y(t)|^2 dt - (\lambda_0 + 1)\omega \int_{\alpha_n}^{\alpha_m} |y'(t)|^2 dt \\ & = (1 - (\lambda_0 + 1)\omega) \int_{\alpha_n}^{\alpha_m} |y(t)|^2 dt - (\lambda_0 + 1)\omega \int_{\alpha_n}^{\alpha_m} |y'(t)|^2 dt. \end{aligned}$$

Thus, the following inequality holds:

$$(3.11) \quad (1 - (\lambda_0 + 1)\omega) \int_{\alpha_n}^{\alpha_m} (|y(t)|^2 + |y'(t)|^2) dt < \sum_{k=1}^s y'_k(v_k)\bar{y}_k(v_k) - \sum_{k=1}^s y'_{k+1}(v_k)\bar{y}_{k+1}(v_k).$$

Let us simplify the expression on the right hand side of the inequality (3.11), returning to the original variables (see (3.3)):

$$\begin{aligned} (3.12) \quad & \sum_{k=1}^s y'_k(v_k)\bar{y}_k(v_k) - \sum_{k=1}^s y'_{k+1}(v_k)\bar{y}_{k+1}(v_k) \\ & = \sum_{k=1}^s f'_k(v_k)f_k(v_k) - \sum_{k=1}^s f'_{k+1}(v_k)f_{k+1}(v_k) \\ & \quad - i \cdot \sum_{k=1}^s a_k(v_k)f_k^2(v_k) + i \cdot \sum_{k=1}^s a_{k+1}(v_k)f_{k+1}^2(v_k). \end{aligned}$$

The right-hand side of equation (3.6) is real, which means that after integration it will also be real. Therefore, the left side of equation (3.6) before and after integration is also real. Therefore, the expression (3.12) is a real function. Thus, the inequality (3.11) in terms of the source variables will look like this:

$$(3.13) \quad (1 - (\lambda_0 + 1)\omega) \int_{\alpha_n}^{\alpha_m} (|f(t)|^2 + |f'(t)|^2) dt < \sum_{k=1}^s f'_k(v_k) f_k(v_k) - \sum_{k=1}^s f'_{k+1}(v_k) f_{k+1}(v_k).$$

Note that due to $(\lambda_0 + 1)\omega < 1$, there exists a set β_v for which the inequality (3.13) is false. Thus, we have arrived at a contradiction, and, therefore, the theorem is proved.

To summarize, we considered quantum graphs of a certain topological structure (see Definition) with the Schrödinger operator corresponding to the scalar potential of a special form (3.2). A theorem was formulated and proved for the quantum graphs which states that for any fixed eigenvalue, there is a set of constants characterizing the boundary conditions such that the eigenfunction has finitely many zeros. This theorem is not yet the criterion for the discreteness of the spectrum of the Schrödinger operator on a quantum graph in a magnetic field, but allows it to be studied. The obtained result can be useful in physical applications related to the transport properties of nanosystems.

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