

On the spectrum discreteness of the quantum graph Hamiltonian with δ -coupling

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Abstract. The condition on the potential ensuring the discreteness of the spectrum of infinite quantum graph Hamiltonian is considered. The corresponding necessary and sufficient condition was obtained by Molchanov 50 years ago. In the present paper, the analogous condition is obtained for a quantum graph. A quantum graph with infinite leads (edges) or/and infinite chains of vertices such that neighbor ones are connected by finite number of edges and with δ -type conditions at the graph vertices is suggested. The Molchanov-type theorem for the quantum graph Hamiltonian spectrum discreteness is proved.

1. Introduction

Many important properties of nanosystems are predetermined by the spectrum of its Hamiltonian. Particularly, spectrum discreteness shows that the bound states gives one full system in the state space of the corresponding system. The problem investigation starts from classical work of Weyl [1]. Early results are described in [2, 3]. The Hamiltonian spectrum discreteness condition (for the potential on axis or half-axis) was suggested by Molchanov in [15]. This condition becomes necessary and sufficient if we assume that the potential is bounded from below. Later, many authors obtained different sufficient conditions for the discreteness of the spectrum of the Sturm-Liouville or 1D Schrodinger operators[4]-[8]. Good review of results in the field is in [9]. Particularly, there are various necessary or sufficient conditions on locally integrable functions $q(x)$ in order that the

Schrödinger operator $-\frac{d^2}{dx^2} + q(x)$ acting on $C_0^\infty(0, \infty)$ is bounded below and that its Friedrichs

extension has only discrete spectrum. There are also some results for the case of operator valued potentials. In this paper the author reviews known conditions for both cases and presents results that unify and extend the previous work on the subject. Finally the result is applied to the Laplacian on non-compact complete Riemannian manifolds.

One-dimensional Hamiltonians are widely used in physical models. The most effective model of such type is a model of quantum graph (see, e.g., [10], [11]). It is a metric graph with the Schrodinger operator defined at the edges (according the physical motivation) and some coupling conditions at the graph vertices that specify the transition probabilities across the vertices (see, e.g., [12-14]). The problem of the spectrum discreteness is closely related with other classical problem starting from the Sturm theorem - the problem of zeroes of eigenfunctions. At present, it is intensively investigated (see,



e.g., [16]). The Courant theorem with the problem of nodal set counting is not solved in general case yet.

The well-known Molchanov's condition for the potential on the real half-axis (or axis) that guarantees the discreteness of the spectrum of the corresponding one-dimensional Hamiltonian is represented in [17,18]. The main goal of the work is to obtain the similar condition for a special type quantum graph.

2. Molchanov-type theorem

Let Γ be a quantum graph, $V(\Gamma)$ is a set of its vertices and $E(\Gamma)$ is a set of its edges. Let also assume that the graph has finite number of infinite leads (edges) or/and infinite chains of vertices such that neighbor ones are connected by several (finite number) edges. We demand that the lengths of edges of these chains are bounded from below and above by some constants and attend that the periodicity or symmetry properties for this chain isn't needed. Moreover, we assume that after removing of these infinite chains, the graph contains finite number of edges (may be, some of them have infinite lengths).

We assume the following equation at the edges:

$$(H - \lambda I)u(x) = -u''(x) - (\lambda - q(x))u(x) = 0. \quad (1)$$

We deal with the Dirichlet boundary condition at the boundary vertices of the graph and δ -type coupling at the internal graph vertices:

$$\sum_{e \in E_v} \frac{du}{dx_e}(v) = \beta_v u(v), \quad \beta_v > 0, \quad x \in V(\Gamma), \quad (20)$$

where u is continuous on Γ , $V(\Gamma)$ is a set of vertices of Γ , E_v is a set of edges containing vertex v , $\frac{du}{dx_e}(v)$ is a derivative of the solution at the vertex v of the edge e in the outgoing direction from the vertex, β_v , $\beta_v > 0$, are some real positive numbers.

Theorem

Let $q(x)$ be bounded from below, i.e. there exists such constant $c > 0$, that for every x the following inequality takes place: $q(x) > -c$ and satisfy the following conditions on Γ :

Let us take arbitrary $w > 0$. Consider all paths L_a on Γ having lengths w ($|L_a| = w$), where a is the starting point of the path L_a . Let $q(x)$ be such function that (for any w)

$$\lim_{\text{dist}(a, v_0) \rightarrow \infty} \int_{L_a} q(x) dx = \infty. \quad (3)$$

Here v_0 is some fixed vertex of Γ

Then, for every fixed λ there exists a set of β_v , such that any solution $u(x)$ of the problem (1) with the vertices conditions (2) has finite number of zeroes on Γ .

Sketch of the Proof

We will assume that some solution has infinite number of zeroes and will come to a contradiction. Two cases can be considered.

1. Let Γ has finite number of edges. Some of them can have infinite lengths. As we have δ -type conditions at the internal graph vertices and the Dirichlet condition at the boundary vertices, there are no accumulation points at the graph vertices.

If we have an infinite set of zeroes at an edge of finite length, then $u \equiv 0$ on the edge and we can throw off the edge and pose the Dirichlet condition at the end points of this removed edge. At every finite edge one can have finite number of zeroes and due to the finiteness of the number of edges, we have a contradiction. So if we have an infinite number of zeroes on Γ then there is an infinite edge

with this property. For such edge we have the conventional Molchanov's condition for the potential on the real half-axis, i.e. this case simply reduced to the conventional theorem.

2. Let Γ has infinite leads (edges) and infinite chains of vertices such that neighbor ones are connected with finite number of edges.

If the infinite number of zeroes is on the part of the graph that has no chains of rings, the Theorem is proved as in point 1.

Let the infinite number of zeroes be at the infinite chains of vertices such that neighbor ones are connected with finite number of edges.

One can see that adding of a constant to the potential does not change the situation. Hence, it is sufficient to consider the case $q(x) \geq 0$. Let there exist $\lambda = \lambda_0 > 0$ such that there is a solution $u = u(x)$ of the equation (1) that has infinite number of zeroes at the chain.

Evidently, it is impossible for $\lambda = \lambda_0 < 0$ due to the sign of the second derivative of the solution: $u'' = -(\lambda - q(x))u$. Hence, if one has a root α then there are no other roots greater than α .

Let w be a such (small) positive number that $w < \frac{1}{\lambda_0 + 1}$. Let us choose N so large that for $\text{dist}(a, v_0) > N$, where $v_0 \in V(\Gamma)$, one has

$$\int_{L_a} q(x) dx > w(\lambda_0 + 1), \quad (4)$$

where L_a is a path on the graph with the starting point a and $|L_a| = w$. It is possible to choose such N due to the condition (3) for $q(x)$.

In accordance with our assumption that there is an infinite number of zeroes at the chain, there exists some path through the chain to infinity that contains an infinite number of zeroes. Below we will deal with the case of such path. One can enumerate zeroes at this path consequently. Hence, we can choose n for such path that $\text{dist}(\alpha_n, v_0) > N$, and, later, choose m , such that $m > n$ and $\text{dist}(\alpha_m, \alpha_n) > w$. Next, it is possible to suppose that $\text{dist}(\alpha_m, \alpha_n) = Pw$, where P is an integer (due to the conditions $q(x) \geq 0$, $\int_{L_a} q(t) dt > w(\lambda_0 + 1)$).

Let us rewrite equation (1) for $\lambda = \lambda_0$: $u'' = (q(x) - \lambda_0)u$. A difficulty is related with the graph vertices belonging to the path. Let us consider the case. Assume that vertex v belongs to the path. We multiply the both parts by u and integrate over the path from α_n to α_m . To come to a contradiction, we use integration by parts and the mean value theorem. By taking into account inequality (4) and the vertex condition (2), we show that there exists such set of the vertices parameters, β_v , that the following inequality takes place:

$$0 > \{1 - (\lambda_0 + 1)w\} \int_L \{u^2(t) + [u'(t)]^2\} dt,$$

which is impossible as $(\lambda_0 + 1)w < 1$. Hence, we arrive at a contradiction. The proof is complete.

One can use the obtained results for the description of many physical system for which the quantum graph model is appropriate approximation. It is interesting to generalize the result to the decorated quantum graph and to modifications of the Schrodinger operator, e.g., magnetic Schrodinger operator (Landau operator).

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References

- [1] Weyl H. 1908 Über gewöhnliche lineare Differentialgleichungen mit singulären Steilen und ihre Eigenfunktionen. *Nachr. Acad. Wiss. Göttingen. Math. Phys. KI*, 37-64.
- [2] Titchmarsh E. C. 1958 *Eigenfunction expansions* associated with second order differential equations, part 2 (Oxford, Oxford University Press (Clarendon Press)).
- [3] Kats I. S., Krein M. G. 1958 Criteria for the discreteness of the spectrum of a singular string. *Izv. Vyssh. Uchebn. Zaved. Mat.* no. 2, 136–153.
- [4] Ahlbrandt C.D., Hinton D.B., Lewis R.T. 1981. Necessary and sufficient conditions for the discreteness of the spectrum of certain singular differential operators. *Canad. J. Math.* **33**, 229–246.
- [5] Hinton D.B. 1979. Molchanov's discrete spectra criterion for a weighted operator. *Canad. Math. Bull.*, **22**, 425–431.
- [6] Kwong M.K., Zettl A. 1981. Discreteness conditions for the spectrum of ordinary differential operators. *J. Differential Equations*, **40** 53–70.
- [7] Oinarov R., Otelbaev M. 1988. A criterion for a general Sturm–Liouville operator to have a discrete spectrum. *Differential Equations*. **24**, 402–408.
- [8] Curgus B., Read T.T. 2002. Discreteness of the spectrum of second-order differential operators and associated embedding theorems. *J. Differential Equations*, **184** (2), 628 –648.
- [9] Bruning J. 1989 On Schrödinger operators with discrete spectrum. *J. Funct. Anal.* 85 (1) 117-150. DOI: 10.1016/0022-1236(89)90049-9.
- [10] Kuchment P. 2002 Graph model of wave propagation in thin structures *Waves in Random Media* **12** (4), R1-R24.
- [11] Lobanov I.S., Trifanov A.I. and Trifanova E.S. 2013 Genetic algorithm for constructing graphene nanoribbon with given electronic transport properties. *Nanosystems: Phys. Chem. Math.* **4** (4), 512-523.
- [12] Exner P., Keating J. P., Kuchment P., Sunada T. and Teplyaev A. (eds.). 2008. *Analysis on Graphs and Its Applications*. Proc. Symp. Pure Math., 77 (Providence, RI: Amer. Math. Soc.)
- [13] Popov I. Yu., Skorynina A. N., and Blinova I. V.. 2014 On the existence of point spectrum for branching strips quantum graph. *J. Math. Phys.* **55**, 033504, doi: 10.1063/1.4867604
- [14] Popov I.Yu., Smirnov P.I. 2013 Spectral problem for branching chain quantum graph. *Phys. Lett. A*. **377**, 439-442.
- [15] Molchanov A.M.. 1953 On conditions of spectrum discreteness for self-adjoint differential operators of second order. *Proc. Moscow Math. Soc.* **2**, 169-199.
- [16] Band R., Berkolaiko G., Raz H., Smilansky U.. 2012 The number of nodal domains on quantum graphs as a stability index of graph partitions. *Commun. Math. Phys.* **311**, 815–838. DOI: 10.1007/s00220-011-1384-9
- [17] Levitan B.M., Sargsyan I.S.. 1988 *Sturm-Liouville and Dirac operators*, (Moscow: Nauka).
- [18] Eckhardt J., Kostenko A., Malamud M., G. Teschl. 2014 One-dimensional Schrödinger operators with δ' -interactions on Cantor-type sets. *J. Differential Equations* **257** 415–449