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On the ground state of quantum graphs with attractive δ-coupling

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ABSTRACT

We study relations between the ground-state energy of a quantum graph Hamiltonian with attractive δ coupling at the vertices and the graph geometry. We derive a necessary and sufficient condition under which the energy increases with the increase of graph edge lengths. We show that this is always the case if the graph has no branchings while both energy increase and decrease are possible for graphs with a more complicated topology.

1. Introduction

Quantum graphs proved themselves to be a class of systems offering numerous problems interesting from both the physical and mathematical point of view; we refer to the proceedings volume [1] for an extensive bibliography. In this Letter we address the question about relations between the ground-state energy of such a Hamiltonian and geometric properties of the underlying graph, in particular, the lengths of its edges.

A motivation to study this kind of problem is twofold. On the physics side it is, of course, the importance of the ground state as the one to which the system tends to relax when it loses energy due to an interaction with the environment. Since quantum graphs model various real physical systems it is natural to ask about the geometric configurations which are energetically the most favorable. At the same time, mathematically the problem represents a natural extension of the usual spectral-geometry studies of the relations between spectral properties of differential operators and geometry of the manifolds supporting them.

We restrict here our attention to graphs with a finite number of edges, some of which may be semi-infinite, and an attractive δ coupling at the vertices, assuming that the motion at the graph edges away from the vertices is free. Such systems have always a nontrivial negative spectrum with a well-defined ground state; we will ask how the corresponding eigenvalue depends on the finite-edge lengths. First we analyze the case of n attractive δ interactions on the line which can be regarded as a simple chain graph. We will prove that the ground-state energy moves up with increasing distances between the δ potentials in two different ways, by means of a Neumann bracketing and by using the well-known explicit form of such a Hamiltonian resolvent.

After that we will pass to general quantum graphs of the described class. We will show that in such a case the dependence on the edge length is more complicated and its sign is uniquely determined by the form of the ground-state eigenfunction on the particular edge. As long as the graph is a chain we have the monotonicity described above. On the other hand, we will give an example showing that once the graph has at least one nontrivial branching, i.e., a vertex of degree exceeding two, it is possible that the ground-state energy decreases with the increasing edge lengths.

Before proceeding further let us note that relations between quantum graph eigenvalues and edge lengths have been discussed also in other contexts. In particular, Friedlander [2] derived a lower bound on higher eigenvalues for finite graphs in terms of the total graph size. On the other hand, Berkolaiko and Kuchment [3] studied general relations between the point spectrum and the set of edge lengths and coupling constants.

2. A warm-up: δ interactions on a line

Consider first a particle on a line with a finite number of δ-interactions the Hamiltonian of which can be formally written as $-\frac{d^2}{dx^2}+\sum_{j=1}^{n}\alpha_j\delta(x-y_j)$. Following [4] we denote this operator as $-\Delta_{\alpha,Y}$ where $\alpha:=\{\alpha_1,\dots,\alpha_n\}$ and $Y:=\{y_1,\dots,y_n\}$. We suppose

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that all the points y_j are mutually distinct and the interactions are attractive, $\alpha_j < 0$, $j = 1, \ldots, n$. Under this assumption the continuous spectrum of $-\Delta_{\alpha,Y}$ covers the positive halfline and the discrete spectrum in the negative part of the axis is non-empty, in particular, there is a ground-state eigenvalue $\lambda_0 < 0$ with a strictly positive eigenfunction ψ_0[1]; we ask how does λ_0 depend on the geometry of the set Y.

One can conjecture that the ground-state energy decreases when the point interactions are closer to each other. First we prove this claim under an additional assumption.

Proposition 2.1. *Consider sets Y_1, Y_2 of the same cardinality such that $y_{j,1} < y_{j,2} < \cdots < y_{j,n}$, $j = 1, 2$. Let there be an i such that $y_{2,l} = y_{1,l}$ for $l = 1, \ldots, i$ and $y_{2,l} = y_{1,l} + \eta$ for $l = i+1, \ldots, n$. Suppose further the ground-state eigenfunction of the $-\Delta_{\alpha,Y_1}$ satisfies $\psi_0'(y_{1,i}+) < 0$ and $\psi_0'(y_{1,i+1}-) > 0$. Then we have $\min\sigma(-\Delta_{\alpha,Y_1}) \leqslant \min\sigma(-\Delta_{\alpha,Y_2})$ for any $\eta > 0$.*

Proof. Since ψ_0 is positive and satisfies $\psi_0'' = -\lambda_0\psi_0$ between the point interaction sites, the function is convex; by the assumption there is then a point $x_0 \in (y_{1,i}, y_{1,i+1})$ such that $\psi_0'(x_0) = 0$. Consider now the operator $-\tilde{\Delta}_{\alpha,Y_1}$ which acts as $-\Delta_{\alpha,Y_1}$ with the additional splitting[2] Neumann condition at the point x_0; it is obvious that the two operators have the same ground state. Such a Neumann condition separates the two halflines, hence $-\tilde{\Delta}_{\alpha,Y_1}$ can be written as $-\tilde{\Delta}^l_{\alpha,Y_1} \oplus -\tilde{\Delta}^r_{\alpha,Y_1}$. Consider now the operator $-\hat{\Delta}_{\alpha,Y_2} := -\tilde{\Delta}^l_{\alpha,Y_1} \oplus -\Delta_N \oplus -\tilde{\Delta}^r_{\alpha,Y_1}$ where the added operator is the Neumann Laplacian on $L^2(0,\eta)$; it is clear that the latter does not contribute to the negative spectrum, hence $\min\sigma(-\hat{\Delta}_{\alpha,Y_2}) = \min\sigma(-\tilde{\Delta}_{\alpha,Y_1})$. Furthermore, $-\hat{\Delta}_{\alpha,Y_2}$ is obviously unitarily equivalent to $-\Delta_{\alpha,Y_2}$ with added splitting Neumann conditions at the points $x = x_0, x_0 + \eta$, hence the sought result follows from Neumann bracketing [5, Section XIII.15]. □

It is not difficult to see that the assumption about the derivative signs is satisfied if $-\alpha_i, -\alpha_{i+1}$ are large enough or, which is the same by scaling, the distance $y_{i+1} - y_i$ is large enough. However, we can make a stronger claim without imposing restrictions on the ground-state eigenfunction derivatives.

Theorem 2.2. *Suppose again that $\#Y_1 = \#Y_2$ and $\alpha_j < 0$ for all j. Let further $y_{1,i} - y_{1,j} \leqslant y_{2,i} - y_{2,j}$ hold for all i, j and $y_{1,i} - y_{1,j} < y_{2,i} - y_{2,j}$ for at least one pair of i, j, then we have $\min\sigma(-\Delta_{\alpha,Y_1}) < \min\sigma(-\Delta_{\alpha,Y_2})$.*

Proof. We employ Krein's formula [4, Section II.2.1] which makes it possible to reduce the spectral problem at energy k^2 to solution of the secular equation, $\det \Gamma_{\alpha,Y}(k) = 0$, where

$$\big[\Gamma_{\alpha,Y}(k)\big]_{jj'} = -\big[\alpha_j^{-1}\delta_{jj'} + G_k(y_j - y_{j'})\big]_{j,j'=1}^N$$

and $G_k(y_j - y_{j'}) = \frac{i}{2k} e^{ik|y_j - y_{j'}|}$ is the free resolvent kernel. Writing conventionally $k = i\kappa$ with $\kappa > 0$, we have to investigate the *lowest* eigenvalue of $\Gamma_{\alpha,Y}(i\kappa)$ which is, of course, given by

$$\mu_0(\alpha, Y; \kappa) = \min_{|c|=1}\big(c, \Gamma_{\alpha,Y}(i\kappa)c\big)$$

with the minimum taken over all $c \in \mathbb{C}^n$ with $|c| = 1$. It is easy to see that $\mu_0(\alpha, Y; \kappa) > 0$ for all κ large enough; the ground-state energy $-\kappa^2$ corresponds to the *highest* value of κ such that $\mu_0(\alpha, Y; \kappa) = 0$. Since $[\Gamma_{\alpha,Y}(i\kappa)]_{ij} = -\delta_{ij}\alpha_i^{-1} - \frac{1}{2\kappa}e^{-\kappa\ell_{ij}}$, where $\ell_{ij} = |y_i - y_j|$, the quantity to be minimized is explicitly

$$\big(c, \Gamma_{\alpha,Y}(i\kappa)c\big) = \sum_{i=1}^n |c_i|^2\left(-\frac{1}{\alpha_i} - \frac{1}{2\kappa}\right) - 2\sum_{i=1}^n\sum_{j=1}^{i-1} \mathrm{Re}\,\bar{c}_i c_j \frac{e^{-\kappa\ell_{ij}}}{2\kappa}.$$

Next we notice that the eigenfunction corresponding to the ground state, i.e., c for which the minimum is reached can be chosen *strictly positive*; we write symbolically $c > 0$ meaning $c_i > 0$, $i = 1, \ldots, n$. This follows from the fact that the semigroup $\{e^{-t\Gamma_{\alpha,Y}(i\kappa)}: t \geqslant 0\}$ is positivity improving, as a consequence of strict negativity of the off-diagonal elements of $\Gamma_{\alpha,Y}(i\kappa)$ – cf. [5, Section XIII.12 and Problem XIII.97]. This means, in particular, that we have

$$\mu_0(\alpha, Y; \kappa) = \min_{|c|=1,\, c>0}\big(c, \Gamma_{\alpha,Y}(i\kappa)c\big).$$

Take now two configurations, (α, Y) and $(\alpha, \tilde{Y})$ such that $\ell_{ij} \leqslant \tilde{\ell}_{ij}$ and the inequality is strict for at least one pair (i, j). For any fixed $c > 0$ we then have $(c, \Gamma_{\alpha,Y}(i\kappa)c) < (c, \Gamma_{\alpha,\tilde{Y}}(i\kappa)c)$, and consequently, taking a minimum over all such c's we get

$$\mu_0(\alpha, Y; \kappa) < \mu_0(\alpha, \tilde{Y}; \kappa)$$

for *any* $\kappa > 0$ with the obvious consequence for the ground state of $-\Delta_{\alpha,Y}$; the sharp inequality in the last formula holds due to the fact that there is a c for which the minimum is attained. □

Remark 2.3. The argument used above can be extended to other situation. Take for instance, point interactions on a loop, in other words, on a finite interval with periodic boundary conditions. The corresponding Green's function is

$$G_{i\kappa}(x, y) = \frac{\cosh\kappa(\ell - |x - y|)}{2\kappa\sinh\kappa\ell}, \quad |x - y| \leqslant \frac{1}{2}\ell,$$

where ℓ is the length of the loop. Writing the corresponding secular equation we find that expanding the loop without reducing the distances between the neighboring point interaction sites means moving the ground-state energy up.

3. Quantum graphs: setting the problem

After this preliminary let us pass to a more general situation when the particle lives on a graph and the attractive point interaction represent couplings at the graph vertices. Consider a graph Γ consisting of a set of vertices $\mathcal{V} = \{\mathcal{X}_j: j \in I\}$, a set of finite edges $\mathcal{L} = \{\mathcal{L}_{jn}: (j, n) \in I_{\mathcal{L}} \subset I \times I\}$ where $\mathcal{L}_{jn}$ is the edge[3] connecting the vertices $\mathcal{X}_j$ and $\mathcal{X}_n$, and a set of infinite edges $\mathcal{L}_\infty = \{\mathcal{L}_{k\infty}: k \in I_{\mathcal{C}}\}$ attached to them. We regard it as a configuration space of a quantum system with the Hilbert space

$$\mathcal{H} = \bigoplus_{j\in I_{\mathcal{L}}} L^2\big([0, l_j]\big) \oplus \bigoplus_{k\in I_{\mathcal{C}}} L^2\big([0, \infty)\big).$$

the elements of which can be written as columns $\psi = \{(\psi_{jn}: \mathcal{L}_{jn} \in \mathcal{L}\}, \{\psi_{k\infty}: \mathcal{L}_{k\infty} \in \mathcal{L}_\infty\})^T$. We consider the dynamics governed by a Hamiltonian which acts as $-d^2/dx^2$ on each edge. In order to make it a self-adjoint operator, in general boundary conditions

[1] See [4, Theorem II.2.1.3], and also Theorem 3.2 below.

[2] Adding a Neumann condition is understood here in the way standard in bracketing arguments [5, Section XIII.15]. Nevertheless, since Neumann condition is sometimes used as a synonym for Kirchhoff coupling in quantum graphs, we say "splitting" to stress that the functions from the domain of $-\tilde{\Delta}_{\alpha,Y_1}$ are in general discontinuous at x_0.

[3] Without loss of generality we may suppose that each pair of vertices is connected by a single edge; in the opposite case we add extra vertices of degree two to the "superfluous" edges and impose Kirchhoff conditions there.