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 change signs are possible for graphs with a more complicated topology.

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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 [4] 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 favourable. 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 semiinfinite, 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, it is possible that the ground-state decreases with the increasing edge lengths.

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2. A warm-up: δ interactions on line

Consider first a particle on line with a finite number of δ-interactions the Hamiltonian of which can be formally written as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{j=1}^n \alpha_j \delta(x - y_j)$. Following [1] we denote this operator as $-\Delta_{\alpha,Y}$ where $\alpha := \{\alpha_1, \ldots, \alpha_n\}$ and $Y := \{y_1, \ldots, y_n\}$. We suppose 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; 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 $y_{j,1} < y_{j,2} < \ldots < y_{j,n}$. Let there be an i such that $y_{2,j} = y_{1,j}$ for $j = 1, \ldots, i$ and $y_{2,j} = y_{1,j} + \eta$ for $j = i+1, \ldots, n$. Suppose further the ground-state eigenfunction of the $-\Delta_{\alpha,Y_1}$ satisfies $\psi_0'(y_i+) < 0$ and $\psi'(y_{i+1}-) > 0$. Then we have $\min\sigma(-\Delta_{\alpha,Y_1}) \le \min\sigma(-\Delta_{\alpha,Y_2})$ for any $\eta > 0$.*

Proof: Since ψ_0 is positive and satisfies $\psi'' = -\lambda_0\psi$ between the point interaction sites, the function is convex; by the assumption there is then a point $x_0 \in (y_i, y_{i+1})$ 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 Neumann condition at the point x_0; it is obvious that the two operators have the same ground state. The 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 $-\tilde\Delta_{\alpha,Y_2}$ with added Neumann conditions at the points $x = x_0, x_0 + \eta$, hence the sought result follows from Neumann bracketing [9, Sec. 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 $y_{1,i} - y_{1,j} \le y_{2,i} - y_{2,j}$ 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 [1, Sec.II.2.1] which makes it possible to reduce the spectral problem at energy k^2 to solution of the secular equation, $\det\Gamma_{\alpha,Y}(\kappa) = 0$, where

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

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

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

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

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

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 $\{\mathrm{e}^{-t\Gamma_{\alpha,Y}(\kappa)} : t \ge 0\}$ is positivity improving, as a consequence of strict negativity of the off-diagonal elements of $\Gamma_{\alpha,Y}(\kappa)$ — cf. [9], Sec. XIII.12 and Problem XIII.97. This means, in particular, that we have

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

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

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

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

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

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 neighbouring 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 $\mathcal{L} = \{\mathcal{L}_{jn} : (\mathcal{X}_j, \mathcal{X}_n)$ with $(j, n) \in I_{\mathcal{L}} \subset I \times I\}$ and a set of infinite edges $\mathcal{L}_\infty = \{\mathcal{L}_{k\infty} : k \in I_C\}$ attached to them. We regard it as a configuration space of a quantum system with the Hilbert space

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

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

$$(U_j - I)\Psi_j + i(U_j + I)\Psi'_j = 0 \tag{3.1}$$

with unitary matrices U_j have to be imposed at the vertices $\mathcal{X}_j$, where Ψ_j and Ψ'_j are vectors of the functional values and of the (outward) derivatives at the particular vertex, respectively [5, 6, 7]. In other words, the domain of the Hamiltonian consists of all functions in $W^{2,2}(\mathcal{L} \oplus \mathcal{L}_\infty)$ which satisfy the conditions (3.1). We will be interested in the following particular class:

- the internal part of the graphs is finite and so is the number of external edges, $\#I_{\mathcal{L}} < \infty$ and $\#I_C < \infty$
- the coupling at each vertex is of δ type in terminology of [3], i.e. $U_j = \frac{2}{n + i\alpha_j}\mathcal{J} - I$, where $\mathcal{J}$ is the matrix having all the entries equal to one. Explicitly the coupling conditions (3.1) then become

$$\psi_{j,i}(0) = \psi_{j,k}(0) =: \psi_j(0)\,,\ j, k = 1, \dots, n_j\,, \quad \sum_{i=1}^{n_j} \psi'_{j,i}(0) = \alpha_j \psi_j(0)\,, \tag{3.2}$$

  where n_j is the degree of the vertex $\mathcal{X}_j$ and each involved edge is parametrized in such way that $x = 0$ corresponds to the vertex
- for "free endpoints", or vertices of degree one, parametrized by $x_j = l_j$, this in particular means the Robin condition, $\psi'_j(l_j) + \alpha_j \psi_j(l_j) = 0$
- all the couplings involved are non-repulsive, $\alpha_j \le 0$ for all $j \in I$, and at least one of them is attractive, $\alpha_{j_0} < 0$ for some $j_0 \in I$

In such a case it is not difficult to express the quadratic form associated with the quantum-graph Hamiltonian H: it is given by

$$q[\Psi] = \sum_{j\in I_{\mathcal{L}}} \int_0^{l_j} |\psi_j'(x)|^2 \,\mathrm{d}x + \sum_{k\in I_C} \int_{\mathbb{R}_+} |\psi_k'(x)|^2 \,\mathrm{d}x + \sum_{i\in I} \alpha_i |\psi_i(0)|^2, \tag{3.3}$$

where ψ_j, ψ_k are components of the wave function Ψ on the internal and external edges, respectively, and $\psi_i(0)$ are the values at the vertices. The domain of the form consists of L^2 functions which are $W^{1,2}$ on the graph edges and continuous at the vertices.

Proposition 3.1. $\inf\sigma(H) < 0$ *holds under the stated assumptions.*

Proof: If $I_C = \emptyset$ we take a constant function, $\Psi = c$ on Γ which belongs to the form domain because Γ has then a finite length; we get $q[\Psi] \le \alpha_{j_0}|c|^2$. On the other hand, if $I_C \neq \emptyset$, we take Ψ equal to c on the internal part of the graph and to $\psi_k(x) = c\,\mathrm{e}^{-\kappa x}$ on each external semiinfinite edge. The integrals over the internal edges vanish as before and those over external ones are easily evaluated; we get

$$q[\Psi] \le \left(\alpha_{j_0} + \frac{1}{2}\kappa \# I_C\right)|c|^2$$

which can be made negative by choosing κ small enough. □

Theorem 3.2. *In addition, let* Γ *be connected, then the bottom of the spectrum* $\lambda_0 = \inf\sigma(H)$ *is a simple isolated eigenvalue. The corresponding eigenfunction* $\Psi^{(0)}$ *can be chosen strictly positive on* Γ *being convex on each edge.*

Proof: Consider a disjoint graph with all the vertex couplings changed to Dirichlet conditions. In such a case the spectrum is positive; it is discrete if $I_C = \emptyset$ and equal to $\mathbb{R}_+$ otherwise. By Krein's formula [8, Proposition 2.3], the original operator differs from the Dirichlet decoupled one by a finite-rank perturbation in the resolvent, hence their essential spectra are the same by Weyl's theorem and the negative spectrum of H may consist at most of a finite number of eigenvalues of finite multiplicity; by the previous proposition it is nonempty and the ground-state eigenvalue exists.

The ground state positivity follows, e.g., from a quantum-graph modification of the Courant theorem [2]. The eigenfunction being positive and its component $\psi_j^{(0)}$ at the jth edge twice differentiable away of the vertices, we have $(\psi_j^{(0)})'' = -\lambda_0\psi_j^{(0)} > 0$, which means the convexity. □

In fact, one can say more about the ground-state eigenfunction because the corresponding Schrödinger equation can be solved explicitly. Writing the spectral threshold as $\lambda_0 = -\kappa^2$ we see that the eigenfunction component on each edge is a linear combination of $\mathrm{e}^{\kappa x}$ and $\mathrm{e}^{-\kappa x}$. Since we are free to choose the edge orientation, each component has one of the following three forms,

$$\psi_j^{(0)}(x) = \begin{cases} c_j \cosh\kappa(x+d_j) & \dots \quad d_j \in \mathbb{R} \\ c_j\, e^{\kappa(x+d_j)} & \dots \quad d_j \in \mathbb{R} \\ c_j \sinh\kappa(x+d_j) & \dots \quad d_j > 0 \end{cases} \tag{3.4}$$

where c_j is a positive constant. For further purposes we introduce *edge index*

$$\sigma_j := \begin{cases} +1 & \dots \quad \psi_j^{(0)}(x) = c_j \cosh\kappa(x+d_j) \\ 0 & \dots \quad \psi_j^{(0)}(x) = c_j\, e^{\kappa(x+d_j)} \\ -1 & \dots \quad \psi_j^{(0)}(x) = c_j \sinh\kappa(x+d_j) \end{cases} \tag{3.5}$$

4. Monotonicity proof by a scaling argument

From now on we consider connected graphs only which we can do without loss of generality, since otherwise we deal with each connected component separately. By Theorem 3.2 the graphs Hamiltonian H then has a simple ground state with positive eigenfunction. We can make the following claim.

Theorem 4.1. *Under the stated assumptions, consider graphs Γ and $\tilde\Gamma$ with the same topology differing possibly in the inner edge lengths. Let H and $\tilde H$ be the corresponding Hamiltonians with the same couplings in the respective vertices, and λ_0 and $\tilde\lambda_0$ the corresponding ground-state eigenvalues. Suppose that $\sigma_j\tilde l_j \le \sigma_j l_j$ holds all $j \in I_C$, then $\tilde\lambda_0 \le \lambda_0$; the inequality is sharp if $\sigma_j\tilde l_j < \sigma_j l_j$ holds for at least one $j \in I_C$.*

Proof: It is obviously sufficient to compare graphs differing just by the length of a single inner edge corresponding to a fixed index value $j \in I_C$. We choose a finite-length segment $J \equiv [a,b]$ in the interior of the jth edge and write Γ as the union of J and $\Gamma_J := \Gamma \setminus J$. Without loss of generality we may choose J in such a way that $b-a > l_j - \tilde l_j$, then $\tilde\Gamma$ can be written as $\Gamma_J := \Gamma \setminus \tilde J$ where $\tilde J$ is obtained by scaling of J with the factor $\xi := |\tilde J||J|^{-1}$ being less than one in case of shrinking and larger than one otherwise.

In order to prove the desired result we have to find a function $\Psi \in L^2(\tilde\Gamma)$ such that the Rayleigh quotient on the tilded graph satisfies

$$\frac{\tilde q[\Psi]}{\|\Psi\|^2} < \lambda_0\,. \tag{4.1}$$

for $\xi < 1$ if $\sigma_j = 1$ and $\xi > 1$ if $\sigma_j = -1$. We construct such a trial function $\tilde\Psi^{(0)}$ in the following way: we put $\tilde\Psi^{(0)}(x) = \Psi^{(0)}(x)$ for $x \in \Gamma_J$ while the jth component on $\tilde J$ is obtained by scaling

$$\tilde\psi_j^{(0)}(\tilde a + \xi y) = \psi_j^{(0)}(a+y) \quad \text{for} \quad 0 \le y \le |J|\,. \tag{4.2}$$

The expression (4.1) can be then easily rewritten in a natural notation as

$$\frac{\tilde q[\tilde\Psi^{(0)}]}{\|\tilde\Psi^{(0)}\|^2} = \frac{a+b\xi^{-1}}{c+d\xi} =: f(\xi)\,, \tag{4.3}$$

where

$$a := q_{\Gamma_J}[\Psi^{(0)}]\,, \quad b := \int_J |(\psi_j^{(0)})'(x)|^2\,\mathrm{d}x\,,$$

and c, d are the part of the squared norm of $\Psi^{(0)}$ corresponding to Γ_J and J, respectively. It is enough to check that $\sigma_j f'(1) = -\sigma_j(bc + 2bd + ad) > 0$. Choosing the ground-state eigenfunction $\Psi^{(0)}$ conventionally with the norm equal to one, we have $c + d = 1$ and $a + b = \lambda_0$, hence the property to be checked is $-\sigma_j(\lambda_0 d + b) > 0$, or more explicitly

$$-\sigma_j\left(\lambda_0\|\psi_j^{(0)}\|_J^2 + \|(\psi_j^{(0)})'\|_J^2\right) > 0\,.$$

Using $\lambda_0 = -\kappa^2$ we find for $\sigma_j = 1$

$$\begin{aligned}\int_J |(\psi_j^{(0)})'(x)|^2\,\mathrm{d}x &= c_j^2\kappa^2\int_J (\sinh\kappa x)^2\,\mathrm{d}x < c_j^2\kappa^2\int_J(\cosh\kappa x)^2\,\mathrm{d}x \\ &= -\lambda_0\int_J |\psi_j^{(0)}(x)|^2\,\mathrm{d}x\,,\end{aligned}$$

and the opposite inequality for $\sigma_j = 1$ where the roles of hyperbolic sine and cosine are interchanged, which is what we have set out to prove. □

5. Discussion

Let us now ask what consequences can one derive from our main result given in Theorem 4.1. First we notice that the graphs without branchings belong all to the same class and one is able to extend to them conclusions of Theorem 2.2 and Remark 2.3. Specifically, we can make the following claim.

Corrolary 5.1. *In the setting of Theorem 4.1 suppose that the graph Γ has no branchings, i.e. the degree of no vertex exceeds two. Then the index of any edge is non-negative being equal to one for any internal edge. Consequently, a length increase of any internal edge moves the ground-state energy up.*

Proof: By assumption a graph without branchings is a chain of edges, either closed into a loop or open; in view of Remark 2.3 we can consider only the latter possibility. It is then obvious that the index of the first and the last edge cannot be negative being +1 and zero for a finite and an infinite edge, respectively. The question is whether one can have a sinh-type solution at some position within the chain. In such a case there would be a vertex in which wavefunction components with different indices have to match. Let us parametrize the chain by a single variable x choosing $x = 0$ for the vertex in question. Suppose that the (non-normalized) ground-state eigenfunction equals $\psi_j(x) = \cosh\kappa(d_1 - x)$ for $x < 0$ and $\psi_{j+1}(x) = c\,\sinh\kappa(d_2 \mp x)$ for $x > 0$. By assumption they are coupled by an attractive δ interaction, hence c is determined by the continuity requirement and $\psi'_{j+1}(0+) - \psi'_j(0-)$ must be negative; recall that the ground-state eigenfunction is positive. However, this expression equals $\mp\kappa\cosh\kappa(d_1 \pm d_2)/\sinh\kappa d_2$, hence the needed match is impossible for a sinh solution decreasing towards the vertex. The same is true for the opposite order of the two solutions, and in a similar way one can check that a negative-index edge cannot neighbour with a semiinfinite one. □

On the other hand, for graphs with a more complicated topology the analogous claim is no longer true. We will illustrate it on a simple example of a star graph with mirror symmetry sketched on Fig. 1. We have plotted here the ground-state energy — in the logarithmic scale to make the effect more visible — as a function of the edge length L_2 and the coupling constant α in the central vertex. We see two regimes here. For weak attractive coupling, $\alpha_{\mathrm{crit}} < \alpha < 0$ where $\alpha_{\mathrm{crit}} \approx -1.09088$, the ground-state energy decreases with increasing L_2 while the opposite is true if $\alpha < \alpha_{\mathrm{crit}}$; at the critical value the energy is independent of L_2 since the solution on the "axial" edge is a pure exponential.

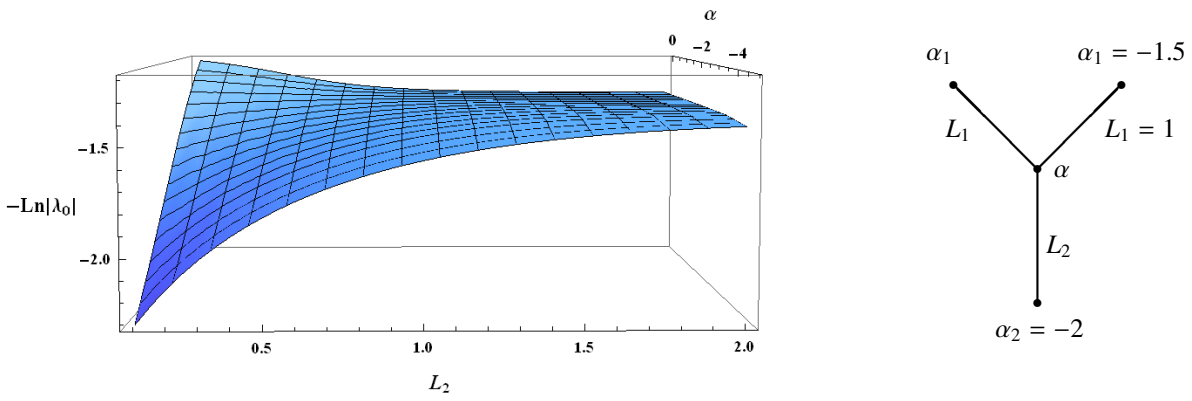

Figure 1: The ground-state energy of sketched star graph as a function of L_2 and α.

The reason why this happens in the example is obvious. The mirror symmetry allows us to decompose the problem into a symmetric part, where the ground state is to be sought, and antisymmetric one which reduced trivially to the Dirichlet problem on a single interval. Using the notation from the proof of Corollary 5.1, the left-hand side of the derivative condition in the symmetric part equals $\psi'_2(0+) - 2\psi'_1(0-)$, hence the argument used there no longer applies. On the other hand, it is not difficult to construct examples without a symmetry in which we have different regimes; an open question is whether one can find a general regime characterization for an arbitrary branching graph.

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