Optimal Potentials for Quantum Graphs

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Abstract. Schrödinger operators on metric graphs with delta couplings at the vertices are studied. We discuss which potential and which distribution of delta couplings on a given graph maximise the ground state energy, provided the integral of the potential and the sum of strengths of the delta couplings are fixed. It appears that the optimal potential if it exists is a constant function on its support formed by a set of intervals separated from the vertices. In the case where the optimal configuration does not exist explicit optimising sequences are presented.

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1. Introduction

Current paper is devoted to the spectral theory of quantum graphs, more precisely of Schrödinger operators on metric graphs with delta couplings at the vertices. Such operators are widely used in both mathematics and physics to model quantum systems where interesting part of the configuration space is localised to a neighbourhood of several intersecting manifolds [5, 18–20]. These models attract attention of mathematicians due to combination of being explicit and exhibiting sophisticated spectral properties at the same time. Spectral theory of quantum graphs is a well-established area of research with numerous interesting papers popping up almost weekly.

One of the most interesting and well-developed areas is spectral estimates, in particular estimates of the spectral gap for Laplace operators on metric graphs [2–4, 14, 18, 19]. Laplace operators on metric graphs with standard vertex conditions always have $\lambda = 0$ as the lowest eigenvalue (ground state energy). Hence, the first non-trivial estimate concerns the second eigenvalue coinciding with the spectral gap. Such estimates are important, since the spectral gap determines the rate of convergence to the equilibrium for the heat evolution.

Considering Schrödinger operators or Laplacians with delta couplings at the vertices one observes that their spectra are asymptotically close to the spectra of standard Laplacians [6, 15], while the lower part of the spectrum may change. The point $\lambda = 0$ is not necessarily an eigenvalue anymore; hence, the role of the spectral gap is played by the energy of the ground state. Explicit universal lower estimates in terms of the positive and negative parts of the interaction were obtained in [12]. The optimal configuration is given by the Laplacian on the interval with Robin conditions at the end points. A similar result is obtained if the graph is fixed. Current paper is devoted to upper estimates, which appear more difficult to obtain. The main reason is that the potential which maximises the ground energy has a tendency to cover the graph uniformly. For example, if no delta couplings are present, then the constant potential $q(x) = Q/\mathcal{L}$ maximises the lowest eigenvalue among all potentials with the fixed integral $Q = \int_{\Gamma} q(x) dx$ [12] ($\mathcal{L}$ is the total length of the graph). If delta couplings at the vertices are present, then the optimal potential appears to be equal to zero near the vertices. The optimal coupling constants at the vertices have a tendency to be distributed uniformly; in particular, in the case where the potential is dominant, the coupling parameters are proportional to the degrees of the vertices (see (32)). One observes an interesting interplay between the potentials in the Schrödinger operator and coupling parameters in the delta vertex conditions.

One of the major difficulties is that the optimal configuration (potential and distribution of coupling parameters) not always exists. One may see a certain parallel to the recent paper [2], where the spectral gap was investigated with respect to the choice of the edge lengths, while the topological graph remained fixed. The authors spoke about *maximisers* and *supremisers* as well as *minimisers* and *infimisers*. We are going to say that either the *optimal configuration* exists or that there is an *optimising sequence*. Note that we always assume that the metric graph is fixed, while we search for the optimal potential and optimal delta couplings. In principle we are facing an optimisation problem in an infinite dimensional space.

Our main results can be formulated as follows:

- The optimisation problem is independent of the topology of the graph; hence, it is enough to study flower graphs (Theorem 6.1).
- If the integral of the potential and the sum of coupling parameters have the same sign, then the optimal configuration exists and is unique. It is described by explicit formulas (17), (18), (20), (21) (Theorems 6.1 and 4.5).
- If the integral of the potential and the sum of coupling parameters have opposite signs, then the optimal configuration does not exist, but the value of the optimal ground state energy can either be given explicitly (Lemma 7.1) or as an eigenvalue of the Laplacian on a flower graph with delta interactions (Lemma 7.2). Optimising sequences are presented.

One may start the investigation by considering single interval which is the simplest metric graph. The problem is trivial (as is shown below) in the case of

Neumann boundary conditions. The case of Dirichlet boundary conditions was formulated as a problem in [21] and resolved in several independent studies [7–9, 11], see also [10]. Arbitrary fixed positive Robin conditions were considered in [13]. We are not able to use these results directly, but they serve as inspiration for our studies.

The paper is organised as follows. After introducing rigorously Schrödinger operator on graphs with delta couplings at the vertices and discussing their elementary spectral properties in Sect. 2 we formulate precisely the optimisation problem in Sect. 3. In Sect. 4 we derive an optimality criterion that will be used to prove that constructed potentials are optimal. This criterion is of general character and may be used in a more general framework, not just for systems described by ordinary differential equations. The optimisation problem is solved for flower graphs. In Sect. 5 we explain how optimal potentials were constructed applying the ideas connected with gluing and cutting graphs. Finally the optimal configuration for arbitrary finite graphs is presented in Sect. 6. The cases when no optimal configuration exists are treated in Sect. 7.

2. Definitions and Elementary Spectral Properties

2.1. Definitions

Consider a set of N compact intervals $e_n = [x_{2n-1}, x_{2n}]$, $n = 1, \dots, N$ on different copies of the real line, called **edges**. The **vertices** v_m , $m = 1, 2, \dots, M$ are defined as a partition of the set $\mathbf{V} = \{x_j\}_{j=1}^{2N}$ of endpoints of the intervals. Then the **metric graph** Γ is the quotient of the (disjoint) union of the edges with respect to the equivalence relation given by the vertices:

$$\Gamma := \bigcup_{n=1}^N \{e_n\} / \sim,$$

where $x \sim y \Leftrightarrow \exists v_m : x, y \in v_m$. We call Γ a **finite compact metric graph**, *metric*, since there is a natural metric induced by the euclidean metric on the intervals, *finite* because the number of edges is finite and *compact* because each of the edges is a compact interval implying that their union is a compact set as well.

We always assume that the graph is **connected**. To each edge corresponds the **length** $\ell_n := |x_{2n} - x_{2n-1}|$ and the sum of the lengths $\mathcal{L}(\Gamma) := \sum_{n=1}^N \ell_n$ is called the **total length** of the graph Γ .

A metric graph is called **flower graph** if it has only one vertex. Any metric graph Γ can be turned into a flower graph F_Γ by identifying all its vertices—the union of all edge end points is considered as a single vertex. The edges of a flower graph are called **petals**. Flower graphs associated with arbitrary metric graphs will play an important role in our studies.

On the edges of any metric graph Γ we consider the differential operator $-\frac{d^2}{dx^2} + q(x)$, with a real absolutely summable potential $q \in L_1(\Gamma)$.

Then the **Schrödinger operator** with delta couplings is defined by this differential expression on the domain

$$\mathcal{D}(L_q^h(\Gamma)) := \left\{ u \in \left(\bigoplus_{n=1}^N \mathcal{W}_2^1(e_n) \right) \cap \mathcal{C}(\Gamma) : -\frac{d^2}{dx^2} u|_{e_n} + qu|_{e_n} \in L_2(e_n), \forall n; \right. \\ \left. \sum_{x_i \in v} \partial u(x_i) = h(v)u(v) \forall v \in V(\Gamma) \right\}, \quad (1)$$

where $\mathcal{C}(\Gamma)$ is the set of continuous functions on Γ and $\partial u(x_i) = (-1)^{i+1} u'(x_i)$ denote normal derivatives at the edge end points and $h : V(\Gamma) \rightarrow \mathbb{R}$ is a real-valued function defined on the vertices. The function h parametrises the delta couplings at the vertices (see, for instance, [5]), it will be called the **singular interaction**, while we refer to q as the **potential**.

2.2. On Spectral Properties of the Schrödinger Operator

Proposition 2.1 (Discreteness of the spectrum [5, 16]). *The spectrum of the Schrödinger operator $L_q^h(\Gamma)$ with a real absolutely summable potential $q \in L_1$ and with real delta vertex conditions is discrete and bounded from below.*

We denote by $Q_{L_q^h(\Gamma)}$ the quadratic form associated with $L_q^h(\Gamma)$, given by

$$Q_{L_q^h(\Gamma)}(u) = \|u'\|^2 + \int_{\Gamma} q(x)|u(x)|^2 dx + \sum_{v \in V(\Gamma)} h(v)|u(v)|^2, \quad (2)$$

on the domain

$$\mathcal{D}(Q_{L_q^h(\Gamma)}) = \left(\bigoplus_{n=1}^N \mathcal{W}_2^1(e_n) \right) \cap \mathcal{C}(\Gamma).$$

It is evident that the domain does not depend neither on the coupling parameters $h(v_m)$ nor on the potential q and it is strictly bigger than the operator domain.

The lowest eigenvalue of any bounded from below operator can be calculated using the Rayleigh quotient [22].

Proposition 2.2 (Rayleigh quotient). *The lowest eigenvalue of $L_q^h(\Gamma)$ is the minimum of the Rayleigh quotient:*

$$\lambda_1(L_q^h(\Gamma)) = \min_{u \in \mathcal{D}(Q_{L_q^h(\Gamma)})} \frac{Q_{L_q^h(\Gamma)}(u)}{\|u\|^2}.$$

The minimiser coincides with the ground state $\psi_1^{L_q^h(\Gamma)}$.

For studying spectral properties the following Perron–Frobenius type theorem is fundamental and its corollary below is employed all along the present article.

Proposition 2.3 (Perron–Frobenius theorem for quantum graphs [17]). *Let Γ be a finite compact connected metric graph on which a Schrödinger operator*

$L_q^h(\Gamma)$ is defined. Then the ground state may be chosen strictly positive $\psi_1 > 0$. Moreover, the corresponding eigenvalue is simple.

Corollary 2.4. *Under the same hypothesis as in Proposition 2.3 let ψ be a real non-negative eigenfunction of $L_q^h(\Gamma)$, then $\psi = \psi_1$, i.e. it is the ground state eigenfunction.*

Proof. Assume that ψ is not the ground state eigenfunction. The orthogonality of the eigenfunctions implies $\langle \psi, \psi_1 \rangle = \int_{\Gamma} \psi \bar{\psi}_1 dx = 0$, which is impossible since both ψ and ψ_1 are strictly positive leading to a contradiction. Hence, ψ is the ground state of $L_q^h(\Gamma)$. $\square$

3. The Optimisation Problem

Given a graph Γ we are interested in understanding which particular form of the potential and which delta couplings maximise the ground state energy λ_1 . We are going to use the following assumptions:

Assumption 3.1. *Given real H and Q we assume that*

1. *the total strength of the potential is fixed:*

$$\int_{\Gamma} q(x) dx = Q; \quad (3)$$

2. *the total strength of the singular interaction is fixed:*

$$\sum_{v \in V} h(v) = H; \quad (4)$$

3. *the potential is sign-definite:* $\begin{cases} q(x) \geq 0 & \text{if } Q \geq 0, \\ q(x) \leq 0 & \text{if } Q \leq 0, \end{cases} \quad \forall x \in \Gamma.$

Extremal properties of the ground state eigenvalue can be described by the function

$$\Lambda(\Gamma, Q, H) := \sup_{\substack{\int q(x) dx = Q \\ \sum_{v \in V} h(v) = H \\ Q q(x) \geq 0}} \lambda_1(L_q^h(\Gamma)) \quad (5)$$

– **the optimal upper bound.**

If the supremum (5) is attained, i.e. there exists a pair (q, h) of singular interaction and potential satisfying Assumption 3.1 and such that $\lambda_1(L_q^h(\Gamma)) = \Lambda(\Gamma, Q, H)$, then we call (q, h) the **optimal configuration** and the associated ground state will be denoted by ψ_1 . If an optimal configuration does not exist (this happens for example if Q and H have different signs), then we need to consider an **optimising sequence** $\{(h_n, q_n)\}_{n \in \mathbb{N}}$ such that the limit $\lim_{n \rightarrow \infty} \lambda_1(L_{q_n}^{h_n}(\Gamma)) = \Lambda(\Gamma, Q, H)$ holds.

Let us motivate all three assumptions introduced above. It is clear that the formulated optimisation problem requires that the integral of q and the sum of delta couplings are bounded from above, since the ground state energy is monotone with respect to both parameters. Why is it necessary to fix each

of these quantities separately? It might look more attractive to fix the total interaction $I := Q + H$. Consider the quadratic form calculated on the trial function $u(x) \equiv 1$

$$Q_{L_q^h(\Gamma)}(1) = Q + H,$$

and hence, we have

$$\lambda_1(L_q^h(\Gamma)) \leq \frac{Q + H}{\mathcal{L}} \Rightarrow \Lambda(\Gamma, Q, H) \leq \frac{Q + H}{\mathcal{L}}. \quad (6)$$

If just the total interaction is fixed, then it is trivial to find the optimal potential and delta couplings:

$$q(x) \equiv I/\mathcal{L}, \quad h \equiv 0,$$

with the constant function being the ground state. Therefore, we need to separate the assumptions 1 and 2. Assumption 3 is needed, since without it any delta interaction may be eliminated by a certain delta-functional sequence of potentials trivialising the problem again. (See Sect. 7 where a similar procedure is implemented.)

4. An Optimality Criterion

4.1. The Criterion

The proof of our main result will be based on a certain optimality criterion, which might look counter-intuitive. In the case of one interval this criterion can be deduced from [13], we manage to adopt it to the case of quantum graphs. To our opinion, this criterion has a much wider domain of applications and can, for example, be used in the case of partial differential equations. In this approach one uses the ground state eigenfunction ψ_1^q which will be always chosen positive. For this eigenfunction we introduce the set where it attains its maximum:

$$M_q := \left\{ x \in \Gamma : \psi_1^q(x) = \max_{y \in \Gamma} \psi_1^q(y) \right\}. \quad (7)$$

The set M_q for optimal potentials on graphs in general is not formed by a discrete set of points, but rather by a union of intervals on the edges.

Lemma 4.1 (Optimality criterion 1). *Let the delta couplings at the vertices (the function h) be fixed. Assume that q^* is a non-negative potential such that*

$$\text{supp } q^* \subseteq M_{q^*} = \left\{ x \in \Gamma : \psi_1^{q^*}(x) = \max_{y \in \Gamma} \psi_1^{q^*}(y) \right\}, \quad (8)$$

then the potential q^ is optimal in the sense that*

$$\lambda_1(L_{q^*}^h(\Gamma)) \geq \lambda_1(L_q^h(\Gamma)) \quad (9)$$

holds for any non-negative potential $q \geq 0$ with the same total strength $\int_\Gamma q^(x)dx = \int_\Gamma q(x)dx$. Moreover, the optimal potential q^* is unique.*

Proof. If normalised the eigenfunction $\psi_1^{q^*}$ is a minimiser of the corresponding quadratic form

$$\lambda_1(L_{q^*}^h(\Gamma)) = Q_{L_{q^*}^h(\Gamma)}(\psi_1^{q^*}) = \min_{\|u\|=1} Q_{L_{q^*}^h(\Gamma)}(u).$$

By the above hypothesis, the evaluation of any other quadratic form $Q_{L_q^h(\Gamma)}$ with $q \neq q^*$ on $\psi_1^{q^*}$ can only be smaller

$$\begin{aligned} Q_{L_{q^*}^h(\Gamma)}(\psi_1^{q^*}) &= \|\psi_1^{q^*}\|^2 + \left(\int_{\Gamma} q^*(x) dx \right) \max_{y \in \Gamma} |\psi_1^{q^*}(y)|^2 + \sum_{v \in V} h(v) |\psi_1^{q^*}(v)|^2 \\ &\geq \|\psi_1^{q^*}\|^2 + \int_{\Gamma} q(x) |\psi_1^{q^*}(x)|^2 dx + \sum_{v \in V} h(v) |\psi_1^{q^*}(v)|^2 \\ &= Q_{L_q^h(\Gamma)}(\psi_1^{q^*}); \end{aligned}$$

then,

$$\lambda_1(L_{q^*}^h) \geq \lambda_1(L_q^h). \quad (10)$$

Assume that $q \neq q^*$, but equality $\lambda_1(L_{q^*}^h) = \lambda_1(L_q^h)$ holds. Then $\psi_1^{q^*}$ is not only a ground state for q^* , but also a ground state for q . But this is impossible, since the potentials are different and $\psi_1^{q^*}$ is not equal to zero (see Proposition 2.3). $\square$

A similar result holds for non-positive potentials and can be proved repeating the arguments:

Lemma 4.2 (Optimality criterion 2). *Let the delta couplings at the vertices (the function h) be fixed. Assume that q^* is a non-positive potential such that*

$$\text{supp } q^* \subseteq m_{q^*} := \left\{ x \in \Gamma : \psi_1^{q^*}(x) = \min_{y \in \Gamma} \psi_1^{q^*}(y) \right\}, \quad (11)$$

then the potential q^ is optimal in the sense that*

$$\lambda_1(L_{q^*}^h(\Gamma)) \geq \lambda_1(L_q^h(\Gamma)) \quad (12)$$

holds for any non-positive potential $q \leq 0$ with the same total strength $\int_{\Gamma} q^(x) dx = \int_{\Gamma} q(x) dx$. Moreover, the optimal potential q^* is unique.*

Remark 4.3. The above lemma can be extended to the case where the potential q is not sign-definite and the integral of the positive and negative components of q are separately fixed, i.e. $\int q_+ dx = Q_+$, $\int q_- dx = Q_-$. In this case the hypothesis reads as follows: $\text{supp } q_+^* \subseteq M_{q^*}$ and $\text{supp } q_-^* \subseteq m_{q^*}$.

4.2. Optimality for the Loop Graph

Let us apply our criterion to the graph formed by just one loop.

Theorem 4.4 (Optimal potential for the loop graph). *On the loop graph $L = [-\frac{\ell}{2}, +\frac{\ell}{2}]$, $v = \{-\frac{\ell}{2}, +\frac{\ell}{2}\}$ with fixed total interactions Q and H such that $HQ \geq 0$ there exists an optimal potential q^* .*

- If $Q, H \geq 0$, then q^* and the corresponding ground state $\psi_1^{q^*}$ are

$$q^*(x) = \begin{cases} 0, \\ k^2, \end{cases} \quad \psi_1^{q^*}(x) = \begin{cases} \cos(k(|x| - \frac{\ell}{2} + \alpha)), & |x| \geq \frac{\ell}{2} - \alpha; \\ 1, & |x| < \frac{\ell}{2} - \alpha; \end{cases} \quad (13)$$

where the parameters α and k are the smallest positive solutions of the system

$$\begin{cases} k^2(\ell - 2\alpha) = Q, \\ 2k \tan(k\alpha) = H. \end{cases} \quad (14)$$

- If $Q, H \leq 0$, then q^* and the corresponding ground state $\psi_1^{q^*}$ are

$$q^*(x) = \begin{cases} 0, \\ -\kappa^2, \end{cases} \quad \psi_1^{q^*}(x) = \begin{cases} \cosh(\kappa(|x| - \frac{\ell}{2} + \alpha)), & |x| \geq \frac{\ell}{2} - \alpha; \\ 1, & |x| < \frac{\ell}{2} - \alpha; \end{cases} \quad (15)$$

where the parameters α and κ are the smallest positive solutions of the system

$$\begin{cases} -\kappa^2(\ell - 2\alpha) = Q, \\ -2\kappa \tanh(\kappa\alpha) = H. \end{cases} \quad (16)$$

Proof. The two cases can be proved in the same way, let us consider the first one $Q, H \geq 0$. The graph has just one vertex; therefore, fixing H we immediately fix $h(v) = H$.

The first equation in (14) comes from the requirement that the potential satisfies assumption (3). The second equation means that the wave function satisfies the vertex conditions, $\sum_{x=\pm\ell/2} \partial \psi_1^{q^*}(x) = H \psi_1^{q^*}(v)$. These two necessary conditions form the system of equations (14), which has a solution in the interval $\alpha \in (0, \ell/2)$. Each of the equations allows one to determine k as a function of $\alpha \in (0, \ell/2)$:

- $k_1(\alpha) = \sqrt{Q/(\ell - 2\alpha)}$ is the unique positive solution to $k^2(\ell - 2\alpha) = Q$,
- $k_2(\alpha)$ is the smallest positive solution to $2k \tan(k\alpha) = H$.

The two functions are plotted in Fig. 1.

The functions are continuous and have the following boundary values on the interval $\alpha \in (0, \ell/2)$:

$$\begin{aligned} k_1 &\xrightarrow{\alpha \rightarrow 0} \sqrt{Q/\ell}, & k_1 &\xrightarrow{\alpha \rightarrow \ell/2} \infty; \\ k_2 &\xrightarrow{\alpha \rightarrow 0} \infty, & k_2 &\xrightarrow{\alpha \rightarrow \ell/2} \text{certain positive number,} \\ && &\text{solution to } 2k \tan(k\ell/2) = H. \end{aligned}$$

The two functions are continuous; hence, there is a solution inside the interval $(0, \ell/2)$.

By construction the wave function is a positive eigenfunction of the operator $L_{q^*}^H(L)$ with $\lambda = k^2$; hence, by Corollary 2.4 it is the ground state. Summing up q^* and $\psi_1^{q^*}$ satisfy the hypothesis of Lemma 4.1 implying that q^* is the unique optimiser for given Q (See Fig. 2). With this we conclude that $\lambda_1(L_{q^*}^H(L)) = \Lambda(L, Q, H)$. $\square$

FIGURE 1. Plot of the functions $k_1(\alpha)$ (blue) and $k_2(\alpha)$ (red) for the following values of the parameters: $\ell = 1$, $Q = 2$ and $H = 1$ (colour figure online)

FIGURE 2. Optimal configurations on the loop graph: in red the potential and the singular interaction, in blue the ground state eigenfunction. Left: $Q, H > 0$, right: $Q, H < 0$ (colour figure online)

4.3. Optimality for Flower Graphs

Developed methods can be applied to determine the optimal configuration for flower graphs. Such graphs have just one vertex and fixing H is equivalent to fixing the vertex conditions. The only difference from the loop is that the potential can be identically equal to zero on certain (short) edges; otherwise, the optimal profile reminds of the one for the loop.

Let us try to guess the optimal configuration for $Q > 0$ and $H > 0$ having in mind our results for the loop graph. Let us parametrise the edges in the graph as $e_n = [-\ell_n/2, \ell_n/2]$. We assume that if $\int_{e_n} q(x)dx =: Q_n \geq 0$ and $\partial\psi_1(-\ell_n/2) + \partial\psi_1(\ell_n/2) := H_n \geq 0$. Then it is natural to guess that the optimal potential and the ground state restricted to e_n coincide with those for the loop and therefore are given by (13).

Consider two edges, say e_1 and e_2 with $Q_1, Q_2 > 0$ and $H_1, H_2 > 0$. We assume that the potential is supported by the intervals $[-\ell_1/2 + \alpha_1, \ell_1/2 - \alpha_1]$ and $[-\ell_2/2 + \alpha_2, \ell_2/2 - \alpha_2]$ and is equal to $k^2 = \lambda$, then we have

$$k^2(\ell_j - 2\alpha_j) = Q_j, \quad j = 1, 2.$$

The ground state is constant on the support of q , it is equal to its maximal value, which will be convenient to assume equal to 1. On the intervals $[-\ell_1/2, -\ell_1/2 + \alpha_1], [\ell_1/2 - \alpha_1, \ell_1/2], [-\ell_2/2, -\ell_2/2 + \alpha_2], [\ell_2/2 - \alpha_1, \ell_2/2]$, the wave function is a solution to the differential equation

$$-\psi''(x) = k^2\psi(x)$$

with the boundary values:

$$\begin{aligned} \psi(-\ell_1/2) &= \psi(\ell_1/2) = \psi(-\ell_2/2) = \psi(\ell_2/2) \\ &= \text{the value of the wave function at the vertex;} \\ \psi(-\ell_1/2 + \alpha_1) &= \psi(\ell_1/2 - \alpha_1) = \psi(-\ell_2/2 + \alpha_2) = \psi(\ell_2/2 - \alpha_2) \\ &= 1 - \text{the maximal value of the wave function;} \\ \psi'(-\ell_1/2 + \alpha_1) &= \psi'(\ell_1/2 - \alpha_1) = \psi'(-\ell_2/2 + \alpha_2) = \psi'(\ell_2/2 - \alpha_2) = 0. \end{aligned}$$

The first condition is due to continuity of the wave function at the vertex, the second condition is needed in order to use the optimality criterion (Lemma 4.1), and the third condition is due to the fact that ψ should be constant on the support of q . Moreover, we want the wave function to be positive, therefore $\alpha_1 = \alpha_2$, and hence, $H_1 = H_2$. Repeating this procedure for any pair of edges we conclude that for all edges with $Q_n > 0$ we have:

$$q_{\alpha,k}(x) = \begin{cases} 0, \\ k^2, \end{cases} \quad \psi_{\alpha,k}(x) = \begin{cases} \cos(k(|x| - (\alpha - \frac{\ell_n}{2}))), & |x| \geq \alpha - \frac{\ell_n}{2}; \\ 1, & |x| \leq \alpha - \frac{\ell_n}{2}, \end{cases} \quad (17)$$

where α is a common real parameter. In what follows we assume that for all edges with $\ell_n > 2\alpha$ the total potential is positive $Q_n > 0$ and the wave functions are given by (17).

If $Q_n = 0$, then the potential is identically zero, and we assume that the wave function is symmetric with respect to the central point on the edge:

$$q_{\alpha,k}(x) \equiv 0, \quad \psi_{\alpha,k}(x) = \frac{\cos k\alpha}{\cos k\ell_n/2} \cos kx, \quad (18)$$

where we adjusted the multiplicative constant so that the wave function is continuous at the vertex. The corresponding H_n is equal to

$$2k \tan k\ell_n/2 = H_n.$$

The function on this interval is less than or equal to 1 (the maximum) only if

$$\frac{\cos k\alpha}{\cos k\ell_n/2} \leq 1 \Rightarrow \ell_n \leq 2\alpha.$$

The potential q and the wave function ψ determined by equations (17) and (18) are defined by the parameters α and k . We calculate the corresponding total potential and total singular interaction and put them equal to Q and H , respectively,

$$\begin{cases} k^2 \sum_{\ell_n \geq 2\alpha} (\ell_n - 2\alpha) = Q, \\ \sum_{\ell_n \geq 2\alpha} 2k \tan k\alpha + \sum_{\ell_n < 2\alpha} 2k \tan k\ell_n/2 = H. \end{cases} \quad (19)$$

It remains to show the existence of a pair of parameters α, k solving the system. Each of the equations (19) allows one to determine k as a function of $\alpha \in (0, \ell_{\max}/2)$, where $\ell_{\max}$ is the length of the longest edge:

- $k_1(\alpha) = \sqrt{\frac{Q}{\sum_{\ell_n \geq 2\alpha} (\ell_n - 2\alpha)}}$ is the unique positive solution to the first equation,
- $k_2(\alpha)$ is the smallest positive solution to the second equation.

As before, these continuous functions have the following limiting values at the end points of the interval $\alpha \in (0, \ell_{\max}/2)$

$$\begin{aligned} k_1 &\xrightarrow{\alpha \rightarrow 0} \sqrt{Q/\mathcal{L}}, \quad k_1 \xrightarrow{\alpha \rightarrow \ell_{\max}/2} \infty; \\ k_2 &\xrightarrow{\alpha \rightarrow 0} \infty, \quad k_2 \xrightarrow{\alpha \rightarrow \ell_{\max}/2} \tilde{k}_2, \end{aligned}$$

where $\tilde{k}_2$ is a positive number, solution to $\sum_{\ell_n} 2k \tan k\ell_n/2 = H$. The two continuous curves must intersect providing a pair (α, k) leading to desired values of Q and H (Fig. 3).

The wave function $\psi_{\alpha,k}$ given by (17) and (18) is a positive eigenfunction for the Schrödinger operator $L_{q_{\alpha,k}}^H(F)$; hence, it is the ground state eigenfunction. The eigenfunction and the potential satisfy the optimality criterion (Lemma 4.1); hence, the constructed potential is optimal.

Similar guess can be used even for the case of negative Q and H . If $\ell_n > 2\alpha$, then the optimal potential and the corresponding ground state are

$$q_{\alpha,\kappa}(x) = \begin{cases} 0, \\ -\kappa^2, \end{cases} \quad \psi_{\alpha,\kappa}(x) = \begin{cases} \cosh(\kappa(|x| - (\alpha - \frac{\ell_n}{2}))), & |x| \geq \alpha - \frac{\ell_n}{2}; \\ 1, & |x| < \alpha - \frac{\ell_n}{2}. \end{cases} \quad (20)$$

If $\ell_n \leq 2\alpha$, then the optimal potential and the corresponding ground state are

$$q_{\alpha,\kappa}(x) \equiv 0, \quad \psi_{\alpha,\kappa}(x) = \frac{\cosh \kappa\alpha}{\cosh \kappa\ell_n/2} \cosh \kappa x, \quad (21)$$

FIGURE 3. Plot of the functions $k_1(\alpha)$ (blue) and $k_2(\alpha)$ (red) for the flower graph composed by three edges with the following values of the parameters: $\ell_1 = 0.1, \ell_2 = 0.2, \ell_3 = 0.7$, $Q = 2$ and $H = 1$. The vertical dashed grey line marks the critical value $\alpha = \ell_1/2, \ell_2/2$ where the derivatives of k_1 and k_2 are discontinuous (colour figure online)

where α and κ solve the system of equations

$$\begin{cases} -\kappa^2 \sum_{\ell_n \geq 2\alpha} (\ell_n - 2\alpha) = Q, \\ -\sum_{\ell_n \geq 2\alpha} 2\kappa \tanh \kappa \alpha - \sum_{\ell_n < 2\alpha} 2\kappa \tanh \kappa \ell_n/2 = H. \end{cases} \quad (22)$$

We may summarise our studies as follows:

Theorem 4.5. *Let F be any finite flower graph, then for arbitrary total potential Q and total singular interaction H , such that $QH > 0$, the optimal potential q^* exists and is unique.*

For $Q > 0$ and $H > 0$ the optimal potential and the corresponding ground state are given by (17) if $\ell_n > 2\alpha$ and by (18) if $\ell_n \leq 2\alpha$, where α and k solve the system of equations (19).

For $Q < 0$ and $H < 0$ the optimal potential and the corresponding ground state are given by (20) if $\ell_n > 2\alpha$ and by (21) if $\ell_n \leq 2\alpha$, where α and k solve the system of equations (22) (Fig. 4).

5. Gluing and Cutting Graphs, or How Could We Guess the Optimal Configuration

To prove Theorem 4.5 we guessed the optimal configuration, which might have surprised the readers. In this section we shall try to explain how did we arrive at that guess. To this end we introduce the operations of *gluing a subset of vertices of a graph* and *cutting a graph at a vertex along a function* and study

FIGURE 4. Four possible optimal configurations on the flower graph with two petals of different lengths: in red the potential and the singular interaction, in blue the ground state eigenfunction (colour figure online)

how do they affect the optimal configurations. In general these techniques go under the name of surgery; for further details see [4, 18, 19].

5.1. Gluing

Definition 5.1 (*Gluing a subset of vertices into one*). Consider a compact finite connected metric graphs Γ on which the Schrödinger operator L_q^h with delta couplings is defined. Let U be a subset of vertices in Γ . Then the **glued graph** $\Gamma' = \sqcup_U \Gamma$ is obtained by joining the vertices $v_m \in U$ into one vertex u ; in other words, the graph Γ' is given by the same set of edges as Γ with the partition of end points given by

$$u \cup \bigcup_{v_m \notin U} v_m. \quad (23)$$

The delta vertex conditions on the new graph are defined by summing the coupling constants for the glued vertices

$$h'(v_m) := \begin{cases} h(v_m) & \text{if } v_m \notin U, \\ \sum_{v_i \in U} h(v_i) & \text{if } v_m = u. \end{cases} \quad (24)$$

The potential q is well defined even on Γ' as an L_1 -function.

The parameters of the Schrödinger operator on the glued graph are chosen in such a way that any function in the domain of $L_q^h(\Gamma)$ attaining equal values at the vertices $v_i \in U$ belongs to the domain of the Schrödinger operator $L_q^{h'}(\Gamma')$ on the glued graph. Hence, we have the following very useful property.

Lemma 5.2. *Let Γ' be a metric graph obtained from a metric graph Γ by gluing the vertices $v_i \in U$, then it holds*

$$\Lambda(\Gamma, Q, H) \leq \Lambda(\Gamma', Q, H), \quad \forall U \subseteq V. \quad (25)$$

Proof. We prove first that

$$\lambda_1(L_q^h(\Gamma)) \leq \lambda_1(L_q^{h'}(\Gamma')) \quad (26)$$

By the definition of gluing we have $\mathcal{C}(\Gamma') \subsetneq \mathcal{C}(\Gamma)$ since continuous functions on Γ may attain different values at different vertices $v_i \in U$. Therefore, the domain $\mathcal{D}$ of the quadratic form for the original graph is larger than the domain $\mathcal{D}'$ for the glued graph, but the expressions $Q(u)$ given by (2) coincide for all $u \in \mathcal{D}$; hence, we conclude

$$\lambda_1(L_q^h(\Gamma)) = \min_{\substack{u \in \mathcal{D} \\ \|u\|=1}} Q(u) \leq \min_{\substack{u \in \mathcal{D}' \\ \|u\|=1}} Q(u) = \lambda_1(L_q^{h'}(\Gamma')).$$

The inequality holds for any $q \in L_1(\Gamma) = L_1(\Gamma')$; therefore, it still holds after taking the supremum over all admissible functions q and h

$$\sup_{\substack{\int_{\Gamma} q = Q, \\ \sum_{v \in V} h(v) = H}} \lambda_1(L_q^h(\Gamma)) \leq \sup_{\substack{\int_{\Gamma'} q = Q, \\ \sum_{v \in V'} h'(v) = H}} \lambda_1(L_q^{h'}(\Gamma')). \quad (27)$$

□

By choosing $U = V(\Gamma)$ we obtain the flower graph $F_{\Gamma} = \sqcup_{V(\Gamma)} \Gamma$ associated with Γ . The following inequality for the optimal bounds holds:

$$\Lambda(\Gamma, Q, H) \leq \Lambda(F_{\Gamma}, Q, H). \quad (28)$$

5.2. Cutting

Definition 5.3 (*Cutting a graph in a vertex along a function*). Let L_q^h be a Schrödinger operator on a compact finite metric graphs Γ with delta couplings at the vertices. Consider any vertex, say v_1 , having degree higher than one. Then any its partition into M_1 equivalence classes

$$v_1 = w_1 \cup w_2 \cup \dots \cup w_{M_1}$$

determines a new graph Γ' with the same set of edges and the vertices determined by the partition

$$w_1 \cup w_2 \cup \dots \cup w_{M_1} \cup v_2 \cup \dots \cup v_M.$$

The delta couplings at the new vertices should naturally satisfy

$$h(v_1) = h(w_1) + h(w_2) + \cdots + h(v_{M_1}),$$

while the couplings at all preserved vertices remain the same.

If in addition we are given a function u on Γ satisfying delta conditions at the vertices, then the coupling parameters at the new vertices should be chosen so that the function u satisfies delta conditions on the new graph Γ'

$$h'(w_m) = \frac{1}{u(v_1)} \sum_{x_i \in w_m} \partial u(x_i), \quad m = 1, \dots, M_1,$$

$$h'(v_m) = h(v_m), \quad m = 2, \dots, M.$$

In the special case $u(v_1) = 0$ we assume Dirichlet conditions at the new vertices. We say that the graph Γ is **cut at the vertex v_1 into Γ' along the function u** .

Notice that the definition of h' depends on the values of u at the vertex v_1 only; in particular, it is invariant under multiplication of the function u by a constant. By Proposition 2.3 the ground state ψ_1 can be chosen real and strictly positive everywhere; therefore, cutting along the ground state is always well defined.

We designed this definition to use cutting to obtain the optimal configuration, but the definition appeared to be useful in a more general context and has already been used in [4].

Lemma 5.4. *Let Γ' be any graph obtained by cutting Γ at some of its vertices along the ground state function ψ_1 of the operator $L_q^h(\Gamma)$. Then ψ_1 is also a ground state function of $L_q^{h'}(\Gamma')$ and $\lambda_1(L_q^{h'}(\Gamma')) = \lambda_1(L_q^h(\Gamma))$.*

Proof. Assume that Γ' is connected, then by construction ψ_1 belongs to the domain of $L_q^{h'}(\Gamma')$ and is a positive function. Hence, by Corollary 2.4, ψ_1 is also the ground state function of $L_q^{h'}(\Gamma')$ and the ground energies of the two operators coincide.

If Γ' is not connected, then restriction of ψ_1 to each connected component is a positive function and satisfies the vertex conditions; hence, it is a ground state of $L_q^{h'}(\Gamma')$, but its multiplicity is equal to the number of connected components. $\square$

We tried to use cutting to get the optimal configuration for an arbitrary flower graph F . Consider any edge e_n forming a loop and let us cut it from F preserving that it is a loop. Of course we cut along the ground state function ψ_1 on F . Then the restriction of ψ_1 to the loop e_n has to be optimal with prescribed $Q_n = \int_{e_n} q^*(x)dx$ and $H_n = (\partial\psi_1(x_{2n-1}) + \partial\psi_1(x_{2n}))/\psi_1(v)$, since if it is not optimal, then making configuration on e_n optimal would increase the ground state for F . Unfortunately we could not prove that H_n is positive, provided that the original H was positive. Therefore, assuming that $Q > 0, H > 0$ we could not guarantee that the optimal configuration on e_n exists. Guessing the formula for the optimal configuration and the ground state we

just assumed that every H_n is positive for every edge. Then from Sect. 4.2 it was easy to get a formula for the optimal potential on every edge. On the other hand, since we have proved that the guessed configuration is optimal, we proved that our guess was correct: one can check that each H_n is positive by looking at the corresponding ground state.

6. Optimality for Arbitrary Graphs

We are in a position to determine the optimal ground energy for an arbitrary finite metric graph. We are going to use gluing and cutting and our knowledge about the optimal configuration for flower graphs. In the case $QH \geq 0$ the optimal configuration exists and we determine it.

Theorem 6.1. *Let Γ be a finite compact connected graph and let F_Γ be its corresponding flower graph. Let the total potential Q and the total singular interaction H be fixed, then we have*

$$\Lambda(\Gamma, Q, H) = \Lambda(F_\Gamma, Q, H). \quad (29)$$

In particular, if q^ is the optimal potential on F_Γ , then (q^*, h') is the optimal configuration on Γ , where h' is obtained by cutting F_Γ into Γ along the flower ground state. Moreover, the same function is a ground state for $L_{q^*}^{h'}(\Gamma)$.*

Proof. We have already proved in Lemma 5.2 that $\Lambda(\Gamma, Q, H) \leq \Lambda(F_\Gamma, Q, H)$; therefore, we need to exclude the inequality.

Assume that the optimal potential q^* on F_Γ exists. Let us cut F_Γ into Γ along the ground state function $\psi_1^{q^*}$ and denote the new coupling function by h' . Then the function $\psi_1^{q^*}$ is also the ground state of $L_{q^*}^{h'}(\Gamma)$ (Lemma 5.4); therefore, $\Lambda(F_\Gamma, Q, H) = \lambda_1(L_{q^*}^H(F_\Gamma)) = \lambda_1(L_{q^*}^{h'}(\Gamma))$. We presented configuration (q^*, h') , which has to be optimal,

$$\begin{aligned} \Lambda(\Gamma, Q, H) &\leq \Lambda(F_\Gamma, Q, H) \\ &\quad \vee \quad \parallel \\ &\lambda_1(L_{q^*}^{h'}(\Gamma)) = \lambda_1(L_{q^*}^H(F_\Gamma)); \end{aligned}$$

hence, the equality holds.

If the optimal configuration on F_Γ does not exist, then consider an approximating sequence q_n and the corresponding sequence of ground states $\psi_1^{q_n}$. By cutting F_Γ into Γ along $\psi_1^{q_n}$ and applying Lemma 5.4 we obtain a sequence (q_n, h'_n) on Γ such that $\lambda_1(L_{q_n}^{h'_n}(\Gamma)) = \lambda_1(L_{q_n}^H(F_\Gamma))$; hence, (q_n, h'_n) is necessarily an approximating sequence of $\Lambda(\Gamma, Q, H)$

$$\begin{aligned} \Lambda(\Gamma, Q, H) &\leq \Lambda(F_\Gamma, Q, H) \\ &\quad \vee \quad \uparrow_{n \rightarrow \infty} \\ &\lambda_1(L_{q_n}^{h'_n}(\Gamma)) = \lambda_1(L_{q_n}^H(F_\Gamma)); \end{aligned}$$

hence, the equality holds again. $\square$

The optimal configuration (q^*, h^*) on an arbitrary graph Γ , if it exists, has the following remarkable properties:

- The optimal potential, $\Lambda(\Gamma, Q, H)$ and the ground state function are independent of the topology of Γ , provided F_Γ is fixed, since the optimal configuration is determined by the flower graph.
- The corresponding ground state attains the same value in all the vertices of the graph. If $Q \geq 0$ and $H > 0$, then the ground state attains its maximum in the middle of a set of longer edges and its minimum in all the vertices. The situation is just opposite if $Q \leq 0$ and $H < 0$.
- Increasing Q (the integral of the potential) the support of the optimal potential on each edge increases as well as the common value of the potential there.
- On a fixed graph Γ we say that the potential is **dominant** over the singular interaction if

$$2N k \tan\left(k \frac{\ell_{\min}}{2}\right) > H, \quad \text{provided } H, Q \geq 0, \quad (30)$$

$$2N \kappa \tanh\left(\kappa \frac{\ell_{\min}}{2}\right) > -H, \quad \text{provided } H, Q \leq 0; \quad (31)$$

where $\ell_{\min}$ is the length of the shortest edge,

$$k = \sqrt{\frac{Q}{\mathcal{L} - N\ell_{\min}}}, \quad \kappa = \sqrt{\frac{-Q}{\mathcal{L} - N\ell_{\min}}}.$$

If the potential is dominant, then it holds:

- The strength of the singular interaction is proportional to the degree of the vertex

$$h^*(v) = \frac{H}{2N} \deg(v). \quad (32)$$

- In the description of the optimal configuration the cases given by formulae (18) and (21) are absent. The optimal potential q^* does not vanish identically on any edge.
- If the potential is not dominant, then the optimal potential vanishes identically on the edges shorter than 2α (Fig. 5).

7. Two Non-optimal Cases

We show that when $Q \cdot H < 0$ then no optimal configuration exists. Two subcases need to be distinguished and are treated in a slightly different manner. The optimising sequences contain delta sequences, and one may use standard theory of singular interactions [1].

Lemma 7.1. *Let Γ be a finite compact connected metric graph. If $0 < -H \leq Q$ or $0 < H \leq -Q$, then there is no optimal configuration and*

$$\Lambda(\Gamma, Q, H) = \frac{Q + H}{\mathcal{L}(\Gamma)}.$$

FIGURE 5. Three possible optimal configurations on a three graph with three edges with different lengths: in red the potential and the singular interaction, in blue the ground state eigenfunction. Plot at the bottom presents the case where the potential is dominant over the singular interaction (colour figure online)

Proof. Assume $0 < -H \leq Q$. It will be convenient to use positive parametrisation so that $H = -\tilde{H}$.

The function $u \equiv 1$ plugged into the quadratic form gives the following estimate for the ground energy (6)

$$Q_{L_q^h}(u) = \frac{Q - \tilde{H}}{\mathcal{L}},$$

but this function does not belong to the domain of the operator; hence, it is not an eigenfunction of any L_q^h . Moreover, the operator L_g^h cannot have $\frac{Q - \tilde{H}}{\mathcal{L}}$ as the lowest eigenvalue, since otherwise $u \equiv 1$ would be a minimiser of the quadratic form and therefore a ground state eigenfunction.

Our goal is to find an approximating sequence (q_j, h_j) fulfilling the constraints with

$$\lambda_1(L_{q_j}^{h_j}) \rightarrow \frac{Q - \tilde{H}}{\mathcal{L}}. \quad (33)$$

To construct such a sequence we are going to use certain approximations of the function $u \equiv 1$, which was our candidate for the ground state. More precisely, let

$$\psi_1^j(x) = \begin{cases} 1, & |x| \leq \ell_n/2 - 1/j, \\ \cosh \kappa_j(|x| - 1/j + \ell_n/2), & |x| > \ell_n/2 - 1/j. \end{cases} \quad (34)$$

Here we assume that j is sufficiently large, so that $\ell_n > 2/j$. We choose the parameters κ_j so that the function satisfies the boundary condition

$$\frac{\partial \psi(x_i)}{\psi(x_i)} = -\frac{\tilde{H}}{2N}.$$

We arrive at the equation

$$\kappa_j \tanh \frac{\kappa_j}{j} = \frac{\tilde{H}}{2N}. \quad (35)$$

The equation has a unique positive solution satisfying the asymptotics

$$\frac{\kappa_j^2}{j} \sim \frac{\tilde{H}}{2N}. \quad (36)$$

We assume that the potential is constant on the intervals $|x| \leq \ell_n/2 - 1/j$ and $|x| > \ell_n/2 - 1/j$. Then the eigenfunction equation

$$-\frac{d^2}{dx^2} \psi_1^j + q(x) \psi_1^j = \lambda_1(L_{q_j}^{h_j}) \psi_1^j$$

gives us

$$q_j(x) = \begin{cases} \lambda_1(L_{q_j}^{h_j}), & |x| \leq \ell_n/2 - 1/j, \\ \lambda_1(L_{q_j}^{h_j}) + \kappa_j^2, & |x| > \ell_n/2 - 1/j. \end{cases} \quad (37)$$

To satisfy the assumption on the potential we need:

$$\lambda_1(L_{q_j}^{h_j}) \mathcal{L} + \frac{\kappa_j^2}{j} 2N = Q,$$

which gives us the ground state energy:

$$\lambda_1(L_{q_j}^{h_j}) = \frac{Q - \frac{\kappa_j^2}{j} 2N}{\mathcal{L}} \rightarrow \frac{Q - \tilde{H}}{\mathcal{L}} = \frac{Q + H}{\mathcal{L}}. \quad (38)$$

The function ψ_1^j is a positive eigenfunction for the operator $L_{q_j}^h$ with

$$h(v) = \frac{H}{2N} \deg(v),$$

and therefore, it is a ground state. Thus, we have constructed an approximating sequence (q_j, h) satisfying (33).

The case $0 < H \leq -Q$ follows similarly after replacing each occurrence of κ_j with ik_j and consequently each hyperbolic function with its trigonometric counterpart. $\square$

Lemma 7.2. *Let Γ be a finite compact connected metric graph. If $0 < -Q \leq H$ or $0 < Q \leq -H$, then no optimal configuration exists and*

$$\Lambda(\Gamma, Q, H) = \lambda_1 \left(L_0^{Q+H}(F_\Gamma) \right).$$

Proof. In Theorem 6.1 it is proved that $\Lambda(\Gamma, Q, H) = \Lambda(F_\Gamma, Q, H)$, so without loss of generality we may assume that the graph is a flower.

The cases $0 < -Q \leq H$ and $0 < Q \leq -H$ are completely equivalent; therefore, we assume that $0 < Q \leq -H$ holds.

We divide the proof into three steps:

1. We show that

$$\Lambda(F, Q, H) \leq \lambda_1 \left(L_0^{Q+H}(F) \right). \quad (39)$$

2. We show that no optimal configuration exists.

3. We construct an optimising sequence q_n such that

$$\lambda_1(L_{q_n}^H(F)) \rightarrow \lambda_1 \left(L_0^{Q+H}(F) \right). \quad (40)$$

Step 1 The ground state function ψ_1 corresponding to $-\kappa^2 = \lambda_1 \left(L_0^{Q+H}(F) \right)$ has already been calculated in (21) and can be chosen equal to

$$\psi_1(x) = \frac{\cosh(\kappa x)}{\cosh(\kappa \ell_n/2)} \quad \text{if } x \in e_n = \left[-\frac{\ell_n}{2}, +\frac{\ell_n}{2} \right]. \quad (41)$$

Note that the function is equal to 1 at the vertex and is strictly smaller than 1 inside the edges.

We are going to use the idea already exploited in the proof of Lemma 4.1: let $q \in L_1$ be any potential with $\int_F q(x) dx = Q$. By construction ψ_1 attains its maximum just at one point—at the central vertex; hence, $Q |\psi_1(v)|^2 \geq \int_F q(x) |\psi_1(x)|^2 dx$ holds. We derive the following inequality for quadratic forms

$$\begin{aligned} Q_{L_0^{Q+H}}(\psi_1) &= \|\psi_1\|^2 + (Q+H)|\psi_1(v)|^2 \\ &\geq \|\psi_1\|^2 + \int_F q(x) |\psi_1(x)|^2 dx + H|\psi_1(v)|^2 \\ &\geq Q_{L_q^H}(\psi_1). \end{aligned} \quad (42)$$

Since ψ_1 is the minimiser for the Rayleigh quotient for $L_0^{Q+H}(F)$ we deduce that $\lambda_1 \left(L_0^{Q+H}(F) \right) \geq \lambda_1 \left(L_q^H(F) \right)$; hence, $\lambda_1 \left(L_0^{Q+H}(F) \right)$ is an upper bound for $\Lambda(F, Q, H)$. On the other hand, $Q_{L_q^H}(u) \geq Q_{L_0^H}(u)$; therefore, for any admissible positive potential q such that $\int_F q dx = Q$ we have

$$\lambda_1 \left(L_0^{Q+H}(F) \right) \geq \lambda_1 \left(L_q^H(F) \right) \geq \lambda_1 \left(L_0^H(F) \right). \quad (43)$$

Step 2 The inequality in (42) is in fact sharp for any potential $q \in L_1$, since its support cannot be just the vertex, but the function ψ_1 is strictly less than 1 inside the edges. Therefore, there is no $q \in L_1$ giving us precisely $\lambda_1 \left(L_0^{Q+H}(F) \right)$.

Step 3 We present an approximating sequence that reaches the calculated upper bound and hence proves optimality of the estimate. Let us consider the following delta sequence q_j different from zero on the first edge e_1 and identically zero on the remaining edges:

$$q_j(x) = \begin{cases} j \frac{Q}{2}, & x \in e_1 \text{ and } |x| \geq \frac{\ell_1}{2} - \frac{1}{j} \\ 0, & \text{otherwise.} \end{cases} \quad (44)$$

Let us introduce the notation $-\kappa_j^2 := \lambda_1 \left(L_{q_j}^H(F) \right) < \frac{H+Q}{\mathcal{L}} < 0$, then the ground state function ψ_1^j is a solution to the equations

$$\begin{aligned} -\psi_1^{j''} &= - \underbrace{\left(j \frac{Q}{2} + \kappa_j^2 \right)}_{=: \tilde{\kappa}_j^2} \psi_1^j, \quad \text{provided } x \in e_1, |x| \geq \frac{\ell_1}{2} - \frac{1}{j}; \\ -\psi_1^{j''} &= -\kappa_j^2 \psi_1^j, \quad \text{otherwise.} \end{aligned}$$

The function ψ_1^j is proportional to a linear combination of hyperbolic functions and therefore can be represented by the hyperbolic cosine up to a phase. We also assume that the function is even with respect to the middle point of each edge:

$$\begin{aligned} \psi_1^j(x) &:= \begin{cases} A_j \cosh(\tilde{\kappa}_j(x + D_j)), & |x| \geq \frac{\ell_1}{2} - \frac{1}{j}, \\ B_j \cosh(\kappa_n x), & |x| < \frac{\ell_1}{2} - \frac{1}{j}; \end{cases} \quad x \in e_1; \\ \psi_1^j(x) &:= C_j^n \cosh(\kappa_n x) \quad x \in e_n \neq e_1. \end{aligned}$$

We normalise the function by assuming that it is equal to 1 at the vertex; then, the values of A_j, B_j and $C_j^n, \forall n \neq 1$ can be calculated taking into account that the function ψ_1^j is continuous everywhere

$$\begin{aligned} \psi_1^j(x) &= \begin{cases} \frac{\cosh(\tilde{\kappa}_j(x + D_j))}{\cosh(\tilde{\kappa}_j(\frac{\ell_1}{2} + D_j))}, & |x| \geq \frac{\ell_1}{2} - \frac{1}{j}, \\ \frac{\cosh(\tilde{\kappa}_j(\frac{\ell_1}{2} - \frac{1}{j} + D_j)) \cosh(\kappa_j x)}{\cosh(\kappa_j(\frac{\ell_1}{2} + D_j)) \cosh(\kappa_j(\frac{\ell_1}{2} - \frac{1}{j}))}, & |x| < \frac{\ell_1}{2} - \frac{1}{j}, \end{cases} \quad \text{if } x \in e_1; \\ \psi_1^j(x) &= \frac{1}{\cosh(\kappa_j \frac{\ell_n}{2})} \cosh(\kappa_j x), \quad \text{if } x \in e_n. \end{aligned}$$

We choose D_j so that the left and right derivatives of ψ_1^j coincide at $\pm x_j \in e_1$, where $x_j := \frac{\ell_1}{2} - \frac{1}{j}$. The function ψ_1^j is continuous and different from zero at these points $\psi_1^j(x_j^-) = \psi_1^j(x_j^+) \neq 0$; hence, continuity of the derivative implies

$$\begin{aligned} \frac{\psi_j'}{\psi_j}(x_j^-) &= \frac{\psi_j'}{\psi_j}(x_j^+) \\ \Rightarrow \kappa_j \tanh(\kappa_j x_j) &= \tilde{\kappa}_j \tanh(\tilde{\kappa}_j(x_j + D_j)), \end{aligned} \quad (45)$$

from which we derive

$$D_j = \frac{1}{\tilde{\kappa}_j} \tanh^{-1} \left(\frac{\kappa_j}{\tilde{\kappa}_j} \tanh(\kappa_j x_j) \right) - x_j.$$

The constructed function should satisfy the delta vertex condition $H = \sum_{x_i \in v} \frac{\partial \psi_j}{\partial \psi_j}(x_i)$ implying

$$M_j(\kappa_j) := -2\tilde{\kappa}_j \tanh \left(\tilde{\kappa}_j \left(\frac{\ell_1}{2} + D_j \right) \right) - 2 \sum_{n=2}^N \kappa_j \tanh \left(\kappa_j \frac{\ell_n}{2} \right) = H, \quad (46)$$

where we introduced the function M_j . The spectral parameter κ_j is the unique solution to the above equation. To show this we prove that $M_j(\kappa)$ is a continuous monotonically decreasing function, such that $M_j(0) > H$ and it is monotonically decreasing to $-\infty$.

To this end consider the following monotonically increasing functions

1. $\tilde{\kappa} = \sqrt{j\frac{Q}{2} + \kappa}$;
2. $\frac{\kappa}{\tilde{\kappa}}$ (to see monotonicity check the derivative $\frac{d}{d\kappa} \frac{\kappa}{\tilde{\kappa}} = \frac{n\frac{Q}{2}}{(n\frac{Q}{2} + \kappa^2)^{\frac{3}{2}}} > 0$);
3. $\tanh, \tanh^{-1}$;
4. $\tilde{\kappa} D_j(\kappa) = \tanh^{-1} \left(\frac{\kappa}{\tilde{\kappa}} \tanh(\kappa x_n) \right) - x_j$.

It follows that $M_j(\kappa)$ is a continuous monotonically decreasing function.

Moreover, each term in the representation of $M_j(\kappa)$ is a monotonically decreasing function and the terms $\kappa \tanh \left(\kappa \frac{\ell_n}{2} \right)$ decrease to $-\infty$. Hence, $M_j(\kappa)$ tends to $-\infty$ as well.

Let us calculate the limit value $M_j(0)$. The sum $2 \sum_{n=2}^N \kappa \tanh \left(\kappa \frac{\ell_n}{2} \right)$ tends to zero as $\kappa \rightarrow 0$. Similarly we have $D_j(0) = -x_j$, implying

$$M_j(0) = -2\sqrt{j\frac{Q}{2}} \tanh \left(\sqrt{j\frac{Q}{2}} \frac{1}{j} \right) > -Q \geq H,$$

where the strict inequality follows from $-\tanh \left(\sqrt{\frac{1}{j} \frac{Q}{2}} \right) > -\sqrt{\frac{1}{j} \frac{Q}{2}}$.

Hence, for all j we have $M_j(0) > H$ which is enough to conclude that the unique solution κ_j exists and is unique.

By construction, $\psi_1^j(x) > 0$ and it solves the eigenvalue equation; hence, by Corollary 2.4 it is the ground state for $L_{q_j}^h(F)$ with the corresponding energy $\lambda_1(L_{q_j}^h(F)) = -\kappa_j^2$. It remains to show that $\lim_{j \rightarrow \infty} -\kappa_j^2 = \lambda_1 \left(L_0^{Q+H}(F_\Gamma) \right)$. Let us prove that as $j \rightarrow \infty$ the functions $M_j(k)$ converge point-wise to the function

$$M(\kappa) := -Q - 2\kappa \sum_{n=1}^N \tanh \left(\kappa \frac{\ell_n}{2} \right).$$

The function M is again continuous monotonically decreasing from $-Q$ to $-\infty$. The unique solution to the equation $M(\kappa) = H$ gives the optimal energy $-\kappa^2 = \lambda_1 \left(L_0^{Q+H}(F_\Gamma) \right)$.

To prove the point-wise convergence consider the difference:

$$M_j(\kappa) - M(\kappa) = -2\tilde{\kappa}_j \tanh \left(\tilde{\kappa}_j \left(\frac{\ell_1}{2} + D_j \right) \right) + 2\kappa \tanh \left(\kappa \frac{\ell_1}{2} \right).$$

We use explicit formula for D_j , or more precisely formula (45) and summation formula for $\tanh$

$$\tanh(\alpha + \beta) = \frac{\tanh(\alpha) + \tanh(\beta)}{1 + \tanh(\alpha) \tanh(\beta)}$$

to get

$$M_j(\kappa) - M(\kappa) = -2 \frac{\kappa \tanh(\kappa x_j) + \tilde{\kappa} \tanh\left(\frac{\tilde{\kappa}}{j}\right)}{1 + \frac{\kappa}{\tilde{\kappa}} \tanh(\kappa x_j) \tanh\left(\frac{\tilde{\kappa}}{j}\right)} + 2\kappa \tanh\left(\kappa \frac{\ell_1}{2}\right) + Q. \quad (47)$$

For any fixed $\kappa > 0$ we have the following explicit limits

$$\begin{aligned} \frac{\kappa}{\tilde{\kappa}} &= \frac{\kappa}{\sqrt{j \frac{Q}{2} + \kappa}} \xrightarrow{j \rightarrow \infty} 0; \quad \frac{\tilde{\kappa}}{j} = \frac{\sqrt{j \frac{Q}{2} + \kappa}}{j} \xrightarrow{j \rightarrow \infty} 0; \quad x_j \xrightarrow{j \rightarrow \infty} \ell_1/2; \\ 2\tilde{\kappa} \tanh\left(\frac{\tilde{\kappa}}{j}\right) &= 2\sqrt{j \frac{Q}{2} + \kappa} \tanh\left(\frac{\sqrt{j \frac{Q}{2} + \kappa}}{j}\right) \xrightarrow{j \rightarrow \infty} Q, \end{aligned}$$

implying

$$M_j(\kappa) \xrightarrow{j \rightarrow \infty} M(\kappa).$$

It follows that solutions to the equation $M_j(\kappa) = H$ converge to the solution of the equation $M(\kappa) = H$. $\square$

8. An Example

In our formulation of the optimisation problem it is important to restrict the singular interactions to the vertices of the graph. If an arbitrary number of vertices could be placed on the graph then an optimal configuration never exists as long as $H \neq 0$ and there always exists an approximating sequence whose ground energy tends to $\frac{H+Q}{2}$.

Example 8.1. Let $I_N, N \in \mathbb{N}$ be the path graph given by N distinct intervals of length $\frac{1}{N}$ each (Fig. 6). Topologically this graph is equivalent to the interval of length one, say $[0, 1]$. The delta interactions may be imposed at the points $x_i = \frac{i}{N}$ with $i = 0, \dots, N$ so that

$$h_N(x_i) = \begin{cases} \frac{H}{2N} & \text{if } i = 0, N; \\ \frac{H}{N} & \text{if } i = 1, \dots, N-1. \end{cases} \quad (48)$$

We have that $\sum_{v \in V(I_N)} h_n(v) = \sum_{i=0}^N h_N(x_i) = H$. The ground state function is given by

$$\psi_{1,N}(x) = \cos\left(k\left(x - \frac{2i+1}{2N}\right)\right) \quad x \in [x_i, x_{i+1}] \quad (49)$$

and the first eigenvalue $\lambda_1(L^{h_N}(I_N)) = k^2$ is given by the smallest positive solution of the equation

$$k \tan\left(\frac{k}{2N}\right) = \frac{H}{2N}. \quad (50)$$

FIGURE 6. Example of $\psi_{1,N}$ (blue) and h (red) on the path graph I_7 for $H \cong 5.5$, $\lambda_1 = 1$ (colour figure online)

From this it appears that $\lim_{N \rightarrow \infty} \lambda_1(L^{h_N}(I_N)) = H$ that is also the upper bound for $\Lambda(I_N, 0, H) \leq H$; therefore,

$$\lim_{N \rightarrow \infty} \Lambda(I_N, 0, H) = H.$$

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