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Leaky quantum graphs: approximations by point-interaction Hamiltonians

P Exner^{1,2} and K Němcová^{1,3}

¹ Nuclear Physics Institute, Academy of Sciences, 25068 Řež near Prague, Czech Republic

² Doppler Institute, Czech Technical University, Břehová 7, 11519 Prague, Czech Republic

³ Institute of Theoretical Physics, FMP, Charles University, V Holešovičkách 2, 18000 Prague, Czech Republic

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Abstract

We prove an approximation result showing how operators of the type $-\Delta - \gamma\delta(x - \Gamma)$ in $L^2(\mathbb{R}^2)$, where Γ is a graph, can be modelled in the strong resolvent sense by point-interaction Hamiltonians with an appropriate arrangement of the δ potentials. The result is illustrated on finding the spectral properties in cases when Γ is a ring or a star. Furthermore, we use this method to indicate that scattering on an infinite curve Γ which is locally close to a loop shape or has multiple bends may exhibit resonances due to quantum tunnelling or repeated reflections.

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1. Introduction

The main aim of this paper is to discuss a limiting relation between two classes of generalized Schrödinger operators in $L^2(\mathbb{R}^2)$. One class is measure-type perturbations of the Laplacian, in particular, we will be interested in potentials which are negative multiples of the Dirac measure supported by a finite graph $\Gamma \subset \mathbb{R}^2$, in other words, they are formally given by the expression

$$-\Delta - \gamma\delta(x - \Gamma) \tag{1.1}$$

with some $\gamma > 0$. We are going to show that such operators can be approximated in the strong resolvent sense by families of point-interaction Hamiltonians [AGHH] with two-dimensional δ potentials suitably arranged.

Stated in this way the problem is an interesting mathematical question; the indicated result will represent an extension of the approximation theorem derived in [BFT] to the two-dimensional situation, which is not straightforward because properties of the δ potentials are dimension-dependent. In addition, we have a strong physical motivation coming from the

fact that Hamiltonians of the type (1.1) are good models of various graph-type nanostructures which in distinction to the usual description [KS] take quantum tunnelling into account—see [Ex1] for a bibliography to this problem.

To investigate such models one has to find spectral properties of the operator (1.1) for various shapes of Γ . This is in general a complicated task even if the original PDE problems are reformulated by means of the generalized Birman–Schwinger principle [BEKŠ] into the solution of an appropriate integral equation. On the other hand, the spectral problem for point-interaction Hamiltonians is reduced in a standard way to the solution of an algebraic equation with coefficients containing values of the free Green function. Hence an approximation of the mentioned type would be of practical importance; our second aim is to illustrate this aspect of the problem with examples.

Let us describe briefly the contents of this paper. In the next section, we collect the needed preliminaries stated in a way suitable for further argument. In section 3 we formulate and prove our main result, which is the approximation indicated above. In the following two sections we discuss examples of two simple graph classes. The first are graphs of the form of a ring, full or open. In this case the spectrum of the operator (1.1) can be found by mode matching [ET] which enables us to compare the approximation with the ‘exact’ result, in particular, to assess the rate of its convergence. In contrast, in section 5 we discuss star-shaped graphs. Here an alternative method for numerical solution of the spectral problem is missing; however, we can derive several conclusions for (an infinite) star analytically and show how the approximation results conform with them. Computations of this type were already performed in [EN] but the number of points used there was too small to provide a reasonable approximation.

In the last section, we address another question which is more difficult and no analytical results are available presently. It concerns the scattering problem on infinite leaky graphs with asymptotically straight ‘leads’. On a heuristic level, it is natural to expect that the states from the negative part of the continuous spectrum can propagate being transversally confined to the graph edges, hence a nontrivial geometry should yield an $N \times N$ on-shell scattering matrix, where N is the number of leads. This remains to be proved, however, and even more difficult will be to compute the S-matrix mentioned above in terms of the graph geometry.

For simplicity we will restrict ourselves to the simplest case when Γ is an infinite asymptotically straight curve, i.e. $N = 2$, without self-intersections. One natural conjecture is that if the distance between the curve points is small somewhere so that Γ is close to a loop shape locally, the system can exhibit resonances due to quantum tunnelling. On the other hand, simple bends are unlikely to produce distinguished resonances; the reason is that the transverse δ coupling in (1.1) has a single bound state, hence there is no analogue here to higher thresholds which give rise to resonances in bent hard-wall tubes [DEM]. To support these conjectures, we have employed the so-called L^2 approach to resonances, which was in the one-dimensional case set on a rigorous ground in [HM]. Specifically, we study the spectrum of a finite segment of Γ as a function of the cut-off position. In the first case we find in this dependence avoided eigenvalue crossings, the more narrow, the smaller the gap to tunnel is, while no such effect is seen in the second case.

On the other hand, tunnelling between arcwise distant points of the graphs is not the only source of resonances. To illustrate this claim, we analyse in our last example a Z-shaped graph with two sharp bends separated by a line segment. We again find avoided crossings the widths of which vary widely as functions of the bending angle. This provides an indirect but convincing indication that the above-described on-shell S-matrix for a bent curve in the shape of a broken line is nontrivial.

2. Preliminaries

2.1. Generalized Schrödinger operators

We start with the definition of Schrödinger operators of the form $-\Delta - \gamma m$ in $L^2(\mathbb{R}^2)$, where m is a finite positive measure on the Borel σ -algebra of Γ , which is assumed to be a non-empty closed subset of \mathbb{R}^2 and also the support of the measure m . Furthermore, γ is a bounded and continuous function, acting from Γ to \mathbb{R}_+ . We suppose that the measure m belongs to the generalized Kato class, in the two-dimensional case meaning that the following condition holds,

$$\limsup_{\varepsilon \rightarrow 0} \sup_{x \in \mathbb{R}^2} \int_{B(x, \varepsilon)} |\log(|x - y|)| m(dy) = 0 \tag{2.1}$$

where $B(x, \varepsilon)$ denotes the circle of radius ε centred at x .

Due to the fact that the measure m belongs to the Kato class, for each $a > 0$ there exists $b \in \mathbb{R}$ such that any ψ from the Schwartz space $\mathcal{S}(\mathbb{R}^2)$ satisfies the inequality

$$\int_{\mathbb{R}^2} |\psi(x)|^2 m(dx) \leq a \int_{\mathbb{R}^2} |\nabla \psi(x)|^2 dx + b \int_{\mathbb{R}^2} |\psi(x)|^2 dx \tag{2.2}$$

as was proved in the paper [SV]. Since $\mathcal{S}(\mathbb{R}^2)$ is dense in $H^1(\mathbb{R}^2)$ we can define a bounded linear transformation

$$\begin{aligned} I_m : H^1(\mathbb{R}^2) &\mapsto L^2(m) \\ I_m \psi &= \psi \quad \forall \psi \in \mathcal{S}(\mathbb{R}^2). \end{aligned}$$

Using this transformation, inequality (2.2) can be extended to the whole $H^1(\mathbb{R}^2)$ with the function ψ on the lhs replaced by $I_m \psi$. By employing the KLMN theorem, see [RS, theorem X.17], we conclude that the quadratic form $q_{\gamma m}$ given by

$$\begin{aligned} D(q_{\gamma m}) &:= H^1(\mathbb{R}^2) \\ q_{\gamma m}(\psi, \phi) &:= \int_{\mathbb{R}^2} \nabla \bar{\psi}(x) \nabla \phi(x) dx - \int_{\mathbb{R}^2} I_m \bar{\psi}(x) I_m \phi(x) \gamma(x) m(dx) \end{aligned} \tag{2.3}$$

is lower semi-bounded and closed in $L^2(\mathbb{R}^2)$. Hence there exists a unique self-adjoint operator $H_{\gamma m}$ associated with the form $q_{\gamma m}$.

The described definition applies to a more general class of measures than we need here. If Γ is a graph consisting of a locally finite number of smooth edges meeting at nonzero angles, i.e. having no cusps, there is another way to define $H_{\gamma m}$, namely via boundary conditions imposed on the wavefunctions. To this aim, consider first the operator $\dot{H}_{\gamma m}$ acting as

$$(\dot{H}_{\gamma m} \psi)(x) = -(\Delta \psi)(x) \quad x \in \mathbb{R}^2 \setminus \Gamma$$

for any ψ of the domain consisting of functions which belong to $H^2(\mathbb{R}^2 \setminus \Gamma)$, and which are continuous at Γ with the normal derivatives having there a jump,

$$\frac{\partial \psi}{\partial n_+}(x) - \frac{\partial \psi}{\partial n_-}(x) = -\gamma \psi(x) \quad x \in \Gamma. \tag{2.4}$$

Then it is straightforward to check that $\dot{H}_{\gamma m}$ is e.s.a. and by Green's formula it reproduces the form $q_{\gamma m}$ on its core, so its closure may be identified with $H_{\gamma m}$ defined above.

An important tool to analyse spectra of such operators is the generalized Birman-Schwinger method. If k^2 belongs to the resolvent set of $H_{\gamma m}$ we put $R_{\gamma m}^k := (H_{\gamma m} - k^2)^{-1}$. The free resolvent R_0^k is defined for $\text{Im } k > 0$ as an integral operator with the kernel

$$G_k(x - y) = \frac{i}{4} H_0^{(1)}(k|x - y|). \tag{2.5}$$

Now we shall use R_0^k to define three other operators. For the sake of generality, suppose that μ, ν are positive Radon measures on \mathbb{R}^2 with $\mu(x) = \nu(x) = 0$ for any $x \in \mathbb{R}^2$. In our case they will be the measure m on Γ and the Lebesgue measure dx on \mathbb{R}^2 in different combinations. By $R_{\nu,\mu}^k$ we denote the integral operator from $L^2(\mu)$ to $L^2(\nu)$ with the kernel G_k , i.e.

$$R_{\nu,\mu}^k \phi = G_k * \phi \mu$$

holds ν -a.e. for all $\phi \in D(R_{\nu,\mu}^k) \subset L^2(\mu)$.

With this notation one can express the resolvent $R_{\gamma m}^k$ as follows [BEKŠ]:

Theorem 2.1. *Let $\text{Im } k > 0$. Suppose that $I - \gamma R_{m,m}^k$ is invertible and the operator*

$$R^k := R_0^k + \gamma R_{dx,m}^k [I - \gamma R_{m,m}^k]^{-1} R_{m,dx}^k$$

from $L^2(\mathbb{R}^2)$ to $L^2(\mathbb{R}^2)$ is everywhere defined. Then k^2 belongs to $\rho(H_{\gamma m})$ and $(H_{\gamma m} - k^2)^{-1} = R^k$.

The invertibility hypothesis is satisfied for all sufficiently large negative k^2 because for such a k^2 the operator norm of $\gamma R_{m,m}(z)$ acting in $L^2(m)$ is less than 1 (see again [BEKŠ]), and a similar result can be proved for the operator norm in $L^\infty(m)$ following [BFT]. Thus from now on we consider $k^2 < 0$ such that both these norms are less than one.

For later considerations it is useful to rewrite operator $H_{\gamma m} = -\Delta - \gamma m$ in the form $-\Delta - \frac{1}{\alpha} \mu$, where we have introduced

$$\mu = \frac{\gamma m}{\int \gamma m} \quad \alpha = \frac{1}{\int \gamma m}. \quad (2.6)$$

Since function γ acquires only non-negative values and m is a positive measure, α is a positive number. The resolvent reads

$$R_{\gamma m}^k = R_0^k + R_{dx,\mu}^k \left(1 - \frac{1}{\alpha} R_{\mu,\mu}^k\right)^{-1} \frac{1}{\alpha} R_{\mu,dx}^k. \quad (2.7)$$

It can be rewritten alternatively as

$$(H_{\gamma m} - z)^{-1} \psi = R_0^k \psi + R_{dx,\mu}^k \sigma \quad (2.8)$$

where $\psi \in L^2(\mathbb{R}^2)$ and $\sigma \in L^2(\mu)$ represents the unique solution to the equation

$$\alpha \sigma - R_{\mu,\mu}^k \sigma = R_{\mu,dx}^k \psi \quad \mu\text{-a.e.} \quad (2.9)$$

Since $R_0^k \psi$ belongs to $H^2(\mathbb{R}^2)$, using Sobolev's embedding theorem we conclude that it has a bounded and continuous version, and therefore σ also has a representative which is bounded and continuous on the set $S_\gamma := \{x \in \Gamma : \gamma(x) \neq 0\}$.

2.2. Schrödinger operators with point interactions

Consider a discrete and finite subset $Y \subset \Gamma$ and the positive constant α defined above. As is well known we cannot regard the operator $H_{Y,\alpha}$ with the interaction supported by Y as before, i.e. as '−Δ + measure'. Instead, we define this operator via its domain: each function $\psi \in D(H_{Y,\alpha})$ behaves in the vicinity of a point $a \in Y$ as follows,

$$\psi(x) = -\frac{1}{2\pi} \log|x - a| L_0(\psi, a) + L_1(\psi, a) + \mathcal{O}(|x - a|) \quad (2.10)$$

where the generalized boundary values $L_0(\psi, a)$ and $L_1(\psi, a)$ satisfy

$$L_1(\psi, a) + 2\pi |Y| \alpha L_0(\psi, a) = 0 \quad (2.11)$$

for any $a \in Y$ with $|Y| := \sharp(Y)$; for a justification of this definition and further properties of the operators $H_{Y,\alpha}$ see, e.g., [AGHH, chap II.4].

The form (2.11) which we have chosen is adapted for the indicated use of these operators in the approximation. In particular, the coupling parameter $|Y|\alpha$ depends linearly on the cardinality of the set Y . However, it is important to stress that our problem differs substantially from its three-dimensional analogue considered in [BFT] where no sign of α played a preferred role. In the two-dimensional setting the coupling parameter tends to $\pm\infty$ in the limit of weak and strong couplings, respectively. Consequently, we will be able to find an approximation for operators (1.1) with *attractive interactions* only.

The Krein formula for the resolvent $(H_{Y,\alpha} - z)^{-1}$ is the basic ingredient in the spectral analysis of the point-interaction Hamiltonians.

Theorem 2.2. *Let $k^2 < 0$ and $\Lambda_{Y,\alpha}(k^2)$ be the matrix $|Y| \times |Y|$ given by*

$$\Lambda_{Y,\alpha}(k^2; x, y) = \frac{1}{2\pi} \left[2\pi|Y|\alpha + \log\left(\frac{ik}{2}\right) + C_E \right] \delta_{xy} - G_k(x - y)(1 - \delta_{xy}) \tag{2.12}$$

where C_E is the Euler constant. Suppose that this matrix is invertible. Then $k^2 \in \rho(H_{Y,\alpha})$ and we have

$$(H_{Y,\alpha} - k^2)^{-1}\psi(x) = R_0^k\psi(x) + \sum_{y,y' \in Y} [\Lambda_{Y,\alpha}(k^2)]^{-1}(y, y')G_k(x - y)R_0^k\psi(y') \tag{2.13}$$

for any $\psi \in L^2(\mathbb{R}^2)$.

One can see easily that the matrix $\Lambda_{Y,\alpha}(k^2)$ is invertible for sufficiently large negative $k^2 = -\kappa^2$. Indeed, the diagonal part is dominated by the term $\frac{1}{2\pi} \log \kappa$, while the non-diagonal elements vanish as $\kappa \rightarrow \infty$, see the asymptotic formula [AS, 9.2.7] for the Hankel function $H_0^{(1)}$. In view of our special choice of the coupling, an alternative way to make the matrix $\Lambda_{Y,\alpha}$ invertible is to take a sufficiently large set Y .

Lemma 2.3. *Let $\text{Im } k > 0$ and $(Y_n)_{n \in \mathbb{N}}$ be a sequence of non-empty finite subsets of S_γ such that $|Y_n| \rightarrow \infty$ as $n \rightarrow \infty$ and the following inequality holds:*

$$\sup_{n \in \mathbb{N}} \frac{1}{|Y_n|} \sup_{x \in Y_n} \sum_{y \in Y_n \setminus \{x\}} G_k(x - y) < \alpha. \tag{2.14}$$

Then there exists a positive C and $n_0 \in \mathbb{N}$ such that the matrix $\Lambda_{Y_n,\alpha}(k^2)$ is invertible and

$$\left\| \left(\frac{1}{|Y_n|} \Lambda_{Y_n,\alpha}(k^2) \right)^{-1} \right\|_{2,2} < C \tag{2.15}$$

holds for all $n \geq n_0$. Here $\|\cdot\|_{p,q}$ means the norm of the map from ℓ^p to ℓ^q ; the specification is superfluous here but it will be useful in the following.

Proof. Let us first decompose the matrix $1/|Y_n|\Lambda_{Y_n,\alpha}(k^2)$ into the diagonal and non-diagonal parts, D_n and R_n , respectively. For n being large enough the diagonal matrix D_n is invertible and its operator norm in $(\mathbb{C}^{|Y_n|}, \|\cdot\|_2)$ converges to α as $n \rightarrow \infty$. Due to the strict inequality in the hypothesis there is an $a < \alpha$ such that the inequality (2.14) holds with α replaced by a . Then the Schur–Holmgren bound [AGHH, app C] yields $\|R_n\|_{2,2} \leq a < \alpha$, which in turn implies that the matrix sum $D_n + R_n$ is invertible for a sufficiently large n . \square

In analogy with the expression (2.8) it is possible to rewrite Krein’s formula (2.13) in the form

$$(H_{Y,\alpha} - k^2)^{-1}\psi(x) = R_0^k\psi(x) + \sum_{y \in Y} G_k(x - y)q_y \tag{2.16}$$

where $q_y, y \in Y_n$ solve the following system of equations,

$$\frac{1}{2\pi} \left[2\pi |Y| \alpha + \log \left(\frac{ik}{2} \right) + C_E \right] q_y - \sum_{y' \in Y, y' \neq y} G_k(y - y') q_{y'} = R_0^k \psi(y) \quad (2.17)$$

for all $y \in Y_n$.

3. Approximation by Schrödinger operators with point interactions

With the above preliminaries we can proceed to the main goal—we will prove that for a chosen generalized Schrödinger operator with an attractive interaction one can find an approximating sequence of point-potential Schrödinger operators under requirements which will be specified below.

The assumption about positions of the point potentials is obvious—loosely speaking, as the sites of potentials are getting denser in the set Γ , they must copy the measure μ . Then we have to specify the coupling-constant behaviour in the approximating operators. We have already mentioned that in the analogous situation in dimension three the coupling constants scale by [BFT] linearly with the number $|Y|$ of point potentials, suggesting the same behaviour here. This requires an explanation, because it is well known that the coupling constants are manifested differently in dimensions three and two; just consider a pair of point potentials and let their distance vary.

To get a hint that the scaling behaviour for the approximation remains nevertheless the same, consider an infinite straight polymer as in [AGHH, III.4], denote the coupling constant by α and the period by $l_0 n^{-1}$. The threshold of the continuous spectrum is given as the unique solution $E = -\kappa^2$ to the implicit equation

$$\alpha = \frac{n}{2l_0\kappa} - \frac{1}{2\pi} \log \frac{2\pi n}{l_0} + \lim_{M \rightarrow \infty} \sum_{m=1}^M \left(\frac{1}{\sqrt{(2\pi m)^2 + (\kappa l_0/n)^2}} - \frac{1}{2\pi m} \right). \quad (3.1)$$

Now let the number n increase. If we want to keep the solution κ preserved as $n \rightarrow \infty$, then α must grow linearly with n ; recall that for $\alpha > 0$ this means that the individual point interactions are becoming *weaker*. This motivates the choice of the coupling constants in the form $|Y|\alpha$ which we made in the boundary condition (2.11).

Now we can prove the announced approximation result.

Theorem 3.1. *Let Γ be a closed and non-empty subset of \mathbb{R}^2 and let m be a finite positive measure on the Borel σ -algebra of Γ with $\text{supp } m = \Gamma$, which belongs to the Kato class. Let $\gamma : \Gamma \rightarrow \mathbb{R}_+$ be a nontrivial bounded continuous function. Choose k with $\text{Im } k > 0$ such that equation (2.9) has a unique solution σ which has a bounded and continuous version on $S_\gamma := \{x \in \Gamma : \gamma(x) \neq 0\}$. Finally, suppose that there exists a sequence $(Y_n)_{n=1}^\infty$ of non-empty finite subsets of S_γ such that $|Y_n| \rightarrow \infty$ and the following relations hold*

$$\frac{1}{|Y_n|} \sum_{y \in Y_n} f(y) \rightarrow \int f \, d\mu \quad (3.2)$$

for any bounded continuous function $f : \Gamma \rightarrow \mathbb{C}$,

$$\sup_{n \in \mathbb{N}} \frac{1}{|Y_n|} \sup_{x \in Y_n} \sum_{y \in Y_n \setminus \{x\}} G_k(x - y) < \alpha \quad (3.3)$$

$$\sup_{x \in Y_n} \left| \frac{1}{|Y_n|} \sum_{y \in Y_n \setminus \{x\}} \sigma(y) G_k(x - y) - (R_{d_{x,\mu}}^k \sigma)(x) \right| \rightarrow 0 \quad (3.4)$$

for $n \rightarrow \infty$. The operators $H_{Y_n, \alpha}$ and H_{γ_m} defined in section 2 then satisfy the relation $H_{Y_n, \alpha} \rightarrow H_{\gamma_m}$ in the strong resolvent sense as $n \rightarrow \infty$.

Proof. Since both Hamiltonians $H_{Y_n, \alpha}$ and H_{γ_m} are self-adjoint it is sufficient to prove the weak convergence, i.e. to check that

$$I_n = (\phi, (H_{Y_n, \alpha} - z)^{-1}\psi - (H_{\gamma_m} - z)^{-1}\psi)_{L^2(\mathbb{R}^2)} \rightarrow 0 \quad \text{as } n \rightarrow \infty$$

holds for arbitrary $\psi, \phi \in L^2(\mathbb{R}^2)$. Using formulae (2.8) and (2.16) for the resolvents we arrive at

$$I_n = \sum_{y' \in Y_n} \frac{1}{|Y_n|} (R_0^k \bar{\phi})(y') [|Y_n| q_{y'} - \sigma(y')] + \frac{1}{|Y_n|} \sum_{y' \in Y_n} (R_0^k \bar{\phi})(y') \sigma(y') - \int (R_{\mu, dx}^k \bar{\phi})(y) \sigma(y) \mu(dy).$$

The sum of the last two terms tends to zero as $n \rightarrow \infty$, which follows from the hypothesis (3.2). Since the function $R_0^k \bar{\phi}$ is continuous and bounded, as we have already mentioned, it is enough to prove the following claim,

$$\frac{1}{|Y_n|} \|v^{(n)}\|_1 \rightarrow 0 \quad \text{as } n \rightarrow \infty$$

for the ℓ^1 norm, where $(v^{(n)})_y := |Y_n| q_y - \sigma(y)$, $y \in Y_n$.

To this end, we employ equations (2.9) and (2.17) and substitute the term $R_{\mu, dx}^k \psi$ in one equation from the other. Equation (2.9) holds μ -a.e., so we must consider continuous representatives of the functions involved here. In this way we get

$$\alpha \sigma(y) - (R_{\mu, \mu}^k \sigma)(y) = \frac{1}{2\pi} \left[2\pi \alpha(y) |Y_n| + \log\left(\frac{ik}{2}\right) + C_E \right] q_y - \sum_{y' \in Y_n, y' \neq y} G_k(y - y') q_{y'}. \tag{3.5}$$

By adding two extra terms to both sides of the equation we arrive at

$$\frac{1}{|Y_n|} \sum_{y' \in Y_n} [\Lambda_{Y_n, \alpha}(k^2; y, y') (q_{y'} |Y_n| - \sigma(y'))] = -\frac{\log(ik/2) + C_E}{2\pi |Y_n|} \sigma(y) + \frac{1}{|Y_n|} \sum_{y' \in Y_n, y' \neq y} G_k(y - y') \sigma(y') - \int G_k(y - y') \sigma(y') \mu(dy').$$

We denote the vector on the rhs by $w^{(n)}$, then the previous formula reads $(1/|Y_n|) \Lambda_{Y_n, \alpha}(z) v^{(n)} = w^{(n)}$. Since we assume that inequality (3.3) holds, lemma 2.3 is applicable here. Therefore, there exists $n_0 \in \mathbb{N}$ such that the matrix $\frac{1}{|Y_n|} \Lambda_{Y_n, \alpha}(z)$ is invertible for all $n > n_0$. Then we can write

$$\frac{1}{|Y_n|} \|v^{(n)}\|_1 \leq \frac{1}{|Y_n|} \left\| \left(\frac{1}{|Y_n|} \Lambda_{Y_n, \alpha}(z) \right)^{-1} \right\|_{\infty, 1} \|w^{(n)}\|_{\infty}.$$

From lemma 2.3 and the relation $\|A\|_{\infty, 1} \leq |Y_n| \|A\|_{2, 2}$, A is an operator acting on $\mathbb{C}^{|Y_n|}$, we conclude that the operator norm in the inequality above is bounded by $|Y_n| C$ for some $C > 0$. Finally, let us look on the norm $\|w^{(n)}\|_{\infty}$: the first term of $(w^{(n)})_y$ converges to zero uniformly w.r.t. y as $n \rightarrow \infty$ (recall that σ is bounded) and hypothesis (3.4) yields that remaining two terms go to zero as well. \square

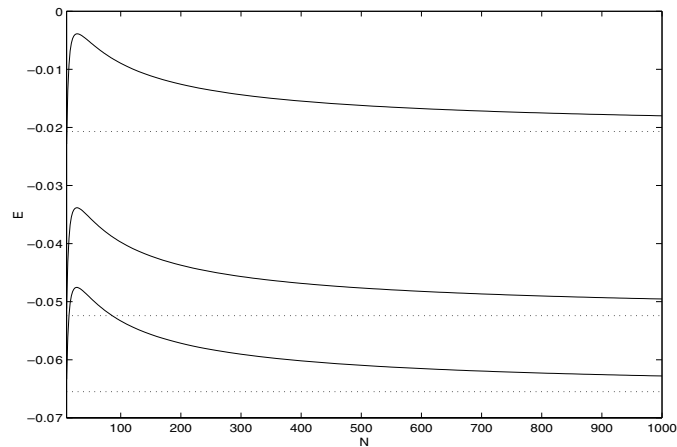


Figure 1. The dependence of eigenvalues of $H_{Y,\alpha}$ on the number of point potentials N for $\gamma = 0.5$ and the ring graph with $R = 10$. The dotted lines are the exact eigenvalues $E_0 = -0.0655$, $E_1 = -0.0524$ and $E_2 = -0.0207$.

4. Soft ring graphs

Let us now pass to examples. The first class of graphs to which we apply the approximation developed in section 3 is rings, both full or open. Since the spectral properties of Hamiltonians with interaction supported by these ring graphs were already explored in the paper [ET]—see also the three-dimensional analogue discussed earlier in [AGS]—this gives us an opportunity to compare the approximation with the ‘exact’ results, in particular, to assess the convergence rate of the approximation.

Consider a circle $\Gamma := \{x \in \mathbb{R}^2 : |x| = R\}$ with the radius $R > 0$ and let γ be a function from Γ to \mathbb{R} such that $\gamma(x) = \gamma \chi_{[0, 2\pi - \theta]}(\varphi)$, where $x = (R, \varphi)$, $\gamma > 0$ and $0 \leq \theta < 2\pi$. The Schrödinger operator with the δ interaction supported by Γ given formally by (1.1) will be denoted by $H_{\gamma,R}$; it can be given meaning in either of the two ways described in section 2. The spectrum and eigenfunctions are found easily in the full ring case, $\theta = 0$, when $H_{\gamma,R}$ is reduced by the angular momentum subspaces. Every eigenstate except the ground state is twice degenerate. In contrast, for a cut ring, $\theta > 0$, the spectrum is simple; the problem can be solved numerically by the mode-matching method [ET].

We start the presentation of the numerical results with the full ring. First, we put $R = 10$ and $\gamma = 0.5$. The discrete spectrum of $H_{\gamma,R}$ consists of three eigenvalues, the ground state corresponds to the angular momentum $l = 0$, the other two correspond to $l = \pm 1, \pm 2$, respectively, and they are twice degenerate; the number of eigenvalues is given by the inequality $\gamma R > 2|l|$. The choice of the approximating point-potential operators $H_{Y_n,\alpha}$ is obvious— N point potentials are spread regularly spaced all over the circle and the coupling constant α equals $N/(2\pi R\gamma)$. The task of finding the eigenvalues E of $H_{Y_n,\alpha}$ means to solve the implicit equation

$$\det \Lambda_{Y,\alpha}(E) = 0. \quad (4.1)$$

We plot the eigenvalues of $H_{Y,\alpha}$ as $N = |Y|$ increases in figure 1.

In the case of a stronger interaction, $\gamma = 1$, one gets a similar picture, just the number of levels rises to five, see figure 2. Note that the convergence of eigenvalues is slower than it

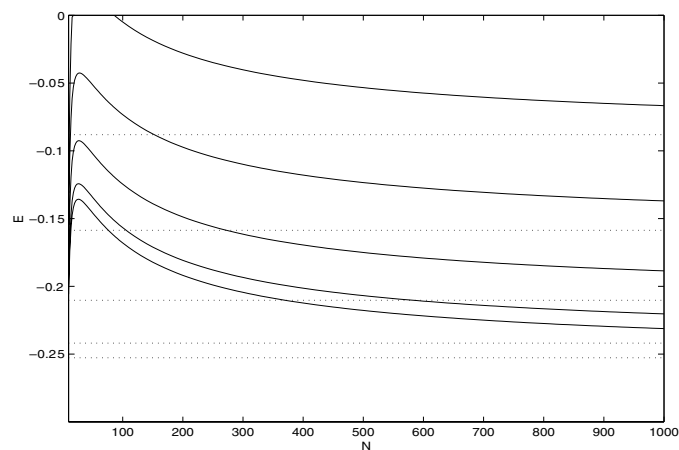


Figure 2. The dependence of eigenvalues of $H_{Y,\alpha}$ on the number of point potentials N for $\gamma = 1$ and the ring graph with $R = 10$. The dotted lines are the exact eigenvalues $E_0 = -0.253$, $E_1 = -0.243$, $E_2 = -0.21$, $E_3 = -0.159$ and $E_4 = -0.0881$.

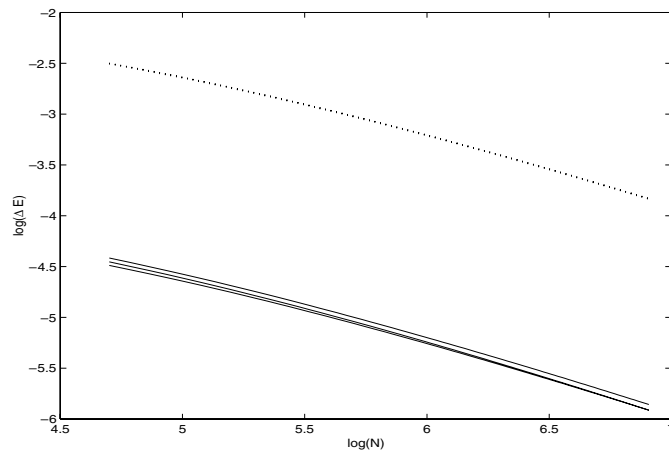


Figure 3. The dependence of the error on the number of point potentials N in the logarithmic scale. The dotted line corresponds to $R = 10$ and $\gamma = 1$ and the solid line corresponds to $R = 10$ and $\gamma = 0.5$.

is for the previous system. To estimate the rate of convergence, we calculate the difference between the exact eigenvalue and the eigenvalue computed using the approximation. The result is shown in figure 3; we observe that the aforementioned difference decays roughly as N^{-a} with a being less than 1.

The approximation by point-potential Schrödinger operators allows us to easily find the eigenfunctions. By [AGHH, theorem II.4.2], they can be written as a linear combination of the free Green functions:

$$\psi_0(x) = \sum_{y \in Y} c_y G_{k_0}(x - y) \quad (4.2)$$

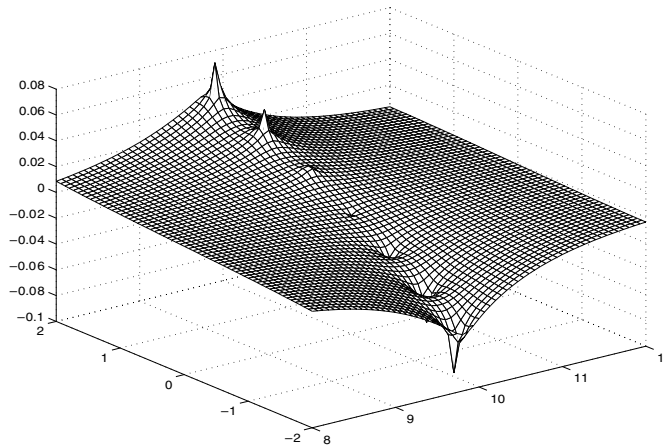


Figure 4. A detail of the wavefunction near the intersection of the circle and one of the nodal lines. It is the wavefunction of the third excited state ($l = 3$) for $R = 10$, $\gamma = 5$ and $|Y| = 100$.

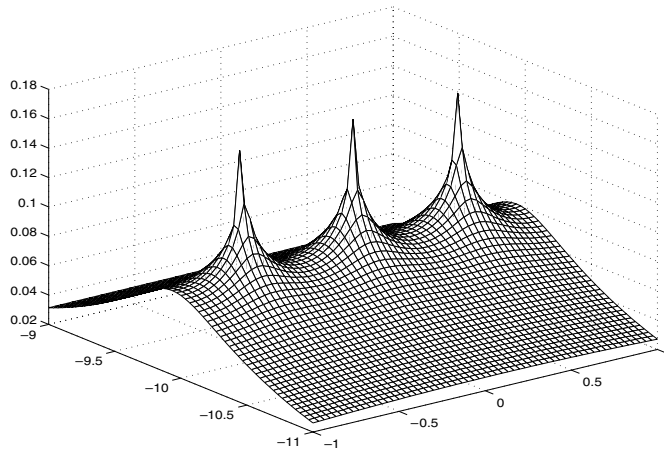


Figure 5. A detail of the wavefunction of the third excited state ($l = 3$) for $R = 10$, $\gamma = 5$ and $|Y| = 100$.

where k_0^2 is the eigenvalue, i.e. $\det \Lambda_{Y,\alpha}(k_0^2) = 0$, and c is the solution to $\Lambda_{Y,\alpha}(k_0^2)c = 0$. The eigenfunctions obtained in this way behave as one expects: they decrease exponentially if moving transversally away from the circle, and for $l > 0$ they copy a sine function if moving along the circle. A closer inspection of the eigenfunctions (4.2) shows, of course, a logarithmic peak at the site of each point potential, as figures 4 and 5 demonstrate. In our opinion, the contributions to energy coming from these spikes are responsible for the slow convergence of the approximation.

Next, we consider an open ring, $\theta = \pi/3$, i.e. one sixth of the perimeter is missing. For example, the fifth excited state for $R = 10$ and $\gamma = 1$ has the energy $E_5 = -0.151$, the corresponding eigenfunction is shown in figure 6. The approximation by 1000 point potentials yields the energy $E'_5 = -0.116$ and the corresponding eigenfunction shown in figure 7.

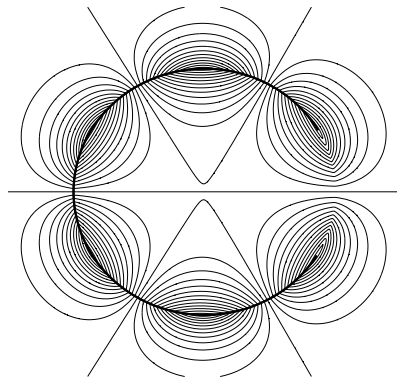


Figure 6. The wavefunction of the fifth excited state of $H_{\gamma,R}$ for $R = 10$, $\gamma = 1$ and $\theta = \pi/3$. The solid line represents the ring Γ .

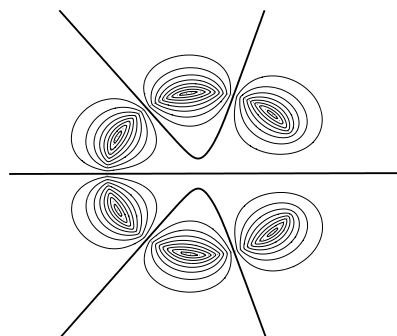


Figure 7. The wavefunction of the fifth excited state of $H_{Y,\alpha}$ for $|Y| = 1000$, which approximates the fifth excited state of $H_{\gamma,R}$ from figure 6. The solid lines represent the nodal lines, the dotted line represents the graph Γ .

5. Star-shaped graphs

Another class of leaky-graph systems to which we will apply the approximation by point-interaction Hamiltonians is the star-graph Hamiltonians where Γ is a collection of segments coupled at a point. In distinction from the previous section no ‘direct’ method to solve the problem is available in this case, and thus the approximation represents the only way to obtain a numerical description of the eigenvalues and eigenfunctions.

First we want to make a remark about the finiteness of such graphs. Our interest concerns primarily infinite stars in which the arms are halflines, in particular, since they support localized states despite the fact that the graph geometry would allow escape to infinity. On the other hand, the above approximation result applies to finite graphs only because it requires $\int \gamma m$ to be finite. Nevertheless, the result can be used, due to the fact that the infinite star Hamiltonian is approximated, again in the strong resolvent sense, by a family of operators with cut-off stars. To justify this claim, it is sufficient to realize that the corresponding family of quadratic forms is by (2.3) monotonic and bounded from below, so that theorem VIII.3.11 of [Ka] applies.

Let us thus discuss in the beginning what can be derived analytically about infinite star graphs. Given an integer $N \geq 2$, consider an $(N - 1)$ -tuple $\beta = \{\beta_1, \dots, \beta_{N-1}\}$ of positive

numbers such that

$$\beta_N := 2\pi - \sum_{j=1}^{N-1} \beta_j > 0.$$

Denote $\vartheta_j := \sum_{i=1}^j \beta_i$, where we put conventionally $\vartheta_0 = 0$. Let L_j be the radial halfline, $L_j := \{x \in \mathbb{R}^2 : \arg x = \vartheta_j\}$, which is naturally parametrized by its arc length $s = |x|$. The support of the interaction is given by $\Gamma \equiv \Gamma(\beta) := \bigcup_{j=0}^{N-1} L_j$.

The star-graph Hamiltonians $H_N(\beta)$ are defined formally by (1.1) as Schrödinger operators with an attractive potential supported by the graph Γ and with the coupling constant γ , and the proper meaning is given to this operator in the way described in section 2.

Remark 5.1. Properties of the operator $H_N(\beta)$ certainly depend on the order of the angles in β . However, the operators obtained from each other by a *cyclic* permutation are obviously unitarily equivalent by an appropriate rotation of the plane.

Let us mention two trivial cases:

Example 5.2. (a) $H_2(\pi)$ corresponding to a straight line can be written as $h_\gamma \otimes I + I \otimes (-\partial_y^2)$, where $h_\gamma = -\partial_x^2 - \gamma\delta(x)$ is the one-centre point-interaction Hamiltonian [AGHH] on $L^2(\mathbb{R})$. Consequently, its spectrum is purely a.c. and equal to $[-\gamma^2/4, \infty)$.

(b) $H_4(\beta_s)$ with $\beta_s = \{\frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{2}\}$ again allows separation of variables being $h_\gamma \otimes I + I \otimes h_\gamma$. Hence the a.c. part of $\sigma(H_4(\beta_s))$ is the same as above, and in addition, there is a single isolated eigenvalue $-\gamma^2/2$ corresponding to the eigenfunction $(2\gamma)^{-1} e^{-\gamma(|x|+|y|)/2}$.

5.1. The essential spectrum

First we note that the essential spectrum of $H_N(\beta)$ does not extend below that of $H_2(\pi)$ corresponding to a straight line.

Proposition 5.3. $\inf \sigma_{\text{ess}}(H_N(\beta)) \geq -\frac{\gamma^2}{4}$ holds for any N and β .

Proof. By Neumann bracketing. We decompose the plane into a finite union

$$P \cup \left(\bigcup_j (S_j \cup W_j) \right) \quad (5.1)$$

where W_j is a wedge of angle β_j , S_j is a halfstrip centred at L_j which is obtained by a Euclidean transformation of $\mathbb{R}^+ \times [\ell, \ell]$ and P is the remaining polygon containing the vertex of Γ . Imposing Neumann boundary conditions at the common boundaries, we get a lower bound to $H_N(\beta)$ by an operator which is a direct sum corresponding to the decomposition (5.1). The wedge parts have an a.c. spectrum in \mathbb{R}^+ while the polygon has a purely discrete spectrum. Finally, the halfstrip spectrum is a.c. again and consists of the interval $[\epsilon(\ell), \infty)$, where $\epsilon(\ell)$ are the lowest eigenvalues of $(-\partial_y^2 - \gamma\delta(y))_N$ on $L^2([-\ell, \ell])$. It is straightforward to see that to any $\eta < -\gamma^2/4$ there is ℓ such that $\epsilon(\ell) > \eta$, and since the decomposition (5.1) can be chosen with ℓ arbitrarily large, the proof is finished. \square

In fact, the essential spectrum is exactly that of a straight line.

Proposition 5.4. $\sigma_{\text{ess}}(H_N(\beta)) = [-\gamma^2/4, \infty)$ holds for any N and β .

Proof. In view of the previous proposition, it is sufficient to check that $\sigma_{\text{ess}}(H_N(\beta)) \supset [-\gamma^2/4, \infty)$. Given a function $\phi \in C_0^\infty([0, \infty))$ with $\|\phi\| = 1$ and $\phi(r) = 1$ in the vicinity of $r = 0$, we construct

$$\psi_n(x; p, x_n) := \frac{1}{n\sqrt{2\gamma}} \phi\left(\frac{1}{n}|x - x_n|\right) e^{-\gamma|x^{(2)}|/2} e^{ipx^{(1)}}$$

with $p \geq 0$ and $x = (x^{(1)}, x^{(2)})$, where the points x_n can be chosen, e.g., as $(n^2, 0)$. It is easy to see that the vectors $\psi_n \rightarrow 0$ weakly as $n \rightarrow \infty$ and that they form a Weyl sequence of $H_N(\beta)$ referring to the value $-\gamma^2/4 + p^2$. This yields the desired result. \square

5.2. The discrete spectrum

The first question naturally concerns the existence of isolated eigenvalues. It follows from two observations of which one is rather simple.

Proposition 5.5. $H_N(\beta) \geq H_{N+1}(\tilde{\beta})$ holds for any N and angle sequence $\tilde{\beta} = \{\beta_1, \dots, \beta_{j-1}, \tilde{\beta}_j^{(1)}, \tilde{\beta}_j^{(2)}, \beta_{j+1}, \dots, \beta_{N-1}\}$ with $\tilde{\beta}_j^{(1)} + \tilde{\beta}_j^{(2)} = \beta_j$.

Proof. It follows directly from the definition by the quadratic form (2.3). \square

On the other hand, the second one is rather nontrivial. It has been proved in [EI] for a wide class of piecewise continuous non-straight curves which includes, in particular, a broken line.

Proposition 5.6. $\sigma_{\text{disc}}(H_2(\beta))$ is nonempty unless $\beta = \pi$.

Combining these two results with the minimax principle (recall that $H_N(\beta)$ is bounded below) we arrive at the following conclusion.

Theorem 5.7. $\sigma_{\text{disc}}(H_N(\beta))$ is nonempty except if $N = 2$ and $\beta = \pi$.

Next one has to ask how many bound states does a star graph support. The answer depends on its geometry. There are situations, however, where their number can be large.

Theorem 5.8. Fix N and a positive integer n . If at least one of the angles β_j is small enough, $\text{card}(\sigma_{\text{disc}}(H_N(\beta))) \geq n$.

Proof. In view of proposition 5.5 it is again sufficient to check the claim for the operator $H_2(\beta)$. Choose the coordinate system in such a way that the two ‘arms’ correspond to $\arg \theta = \pm\beta/2$. We employ the following family of trial functions

$$\Phi(x, y) = f(x)g(y) \tag{5.2}$$

supported in the strip $L \leq x \leq 2L$, with $f \in C^2$ satisfying $f(L) = f(2L) = 0$, and

$$g(y) = \begin{cases} 1 & |y| \leq 2d \\ e^{-\gamma(|y|-2d)} & |y| \geq 2d \end{cases}$$

with $d := L \tan(\beta/2)$. Let us ask under what conditions the value of the shifted energy form

$$q[\Phi] := \|\nabla\Phi\|^2 - \frac{2\gamma}{\cos(\beta/2)} \|f\|^2 + \frac{\gamma^2}{4} \|\Phi\|^2$$

is negative. Since $\|g\|^2 = 4d + \gamma^{-1}$ and $\|g'\|^2 = \gamma$, this is equivalent to

$$\frac{\|f'\|^2}{\|f\|^2} < \gamma^2 \frac{2 \sec \frac{\beta}{2} - \gamma d - \frac{\gamma}{4}}{1 + 4\gamma d}.$$

By the minimax principle for the system there will be at least n isolated eigenvalues provided

$$\left(\frac{\pi n}{d} \tan \frac{\beta}{2}\right)^2 = \inf_{M_n^\perp} \sup_{M_n} \frac{\|f'\|^2}{\|f\|^2} < \gamma^2 \frac{2 \sec \frac{\beta}{2} - \gamma d - \frac{5}{4}}{1 + 4\gamma d}$$

where M_n means an n -dimensional subspace in $L^2([L, 2L])$, i.e., if

$$n^2 < \frac{\gamma^2 d^2}{\pi^2} \left(\cot \frac{\beta}{2}\right)^2 \frac{2 \sec \frac{\beta}{2} - \gamma d - \frac{5}{4}}{1 + 4\gamma d}.$$

Now one should optimize the rhs w.r.t. γd , but for a rough estimate it is sufficient to take a particular value, say $\gamma d = \sec \frac{\beta}{2} - \frac{5}{8}$ which yields

$$n < \frac{1}{16\pi} \cot \frac{\beta}{2} \frac{\left(8 \sec \frac{\beta}{2} - 5\right)^{3/2}}{\left(8 \sec \frac{\beta}{2} - 3\right)^{1/2}} \quad (5.3)$$

it is obvious that the last inequality is for any fixed n satisfied if β is chosen small enough. \square

Corollary 5.9. *Independently of β , $\text{card}(\sigma_{\text{disc}}(H_N(\beta)))$ exceeds any fixed integer for N large enough.*

Remark 5.10. The estimate used in the proof also shows that the number of bound states for a sharply broken line is roughly proportional to the inverse angle,

$$n \gtrsim \frac{3^{3/2}}{8\pi\sqrt{5}} \beta^{-1}$$

as $\beta \rightarrow 0$. This is the expected result, since the number is given by the length of the effective potential well which exists in the region where the two lines are so close that they roughly double the depth of the transverse well.

5.3. The Birman–Schwinger approach

Now we are going to show how the spectral problem for the operators $H_N(\beta)$ can be reformulated in terms of suitable integral operators. We will employ the resolvent formula for measure perturbations of the Laplacian derived in [BEKŠ]. Note that this technique was used in [EI] to derive a result which implies our proposition 5.6.

Since the operators $H_N(\beta)$ are defined by the quadratic form (2.3) they satisfy the generalized Birman–Schwinger principle. If k^2 belongs to the resolvent set of $H_N(\beta)$ we put $R_{\gamma,\Gamma}^k := (H_N(\beta) - k^2)^{-1}$. We already know the Krein-like formula for the resolvent from theorem 2.1, here it has the form

$$R_{\gamma,\Gamma}^k = R_0^k + \gamma R_{\text{dx},m}^k [I - \gamma R_{m,m}^k]^{-1} R_{m,\text{dx}}^k$$

with m denoting the Dirac measure on Γ . One can express the generalized BS principle as follows [BEKŠ]:

Proposition 5.11. $\dim \ker(H_N(\beta) - k^2) = \dim \ker(I - \gamma R_{m,m}^k)$ for any k with $\text{Im } k > 0$.

Consequently, the original spectral problem is in this way equivalent to finding solutions to the equation

$$\mathcal{R}_{\gamma,\Gamma}^k \phi = \phi \quad (5.4)$$

in $L^2(\Gamma)$, where $\mathcal{R}_{\gamma,\Gamma}^\kappa := \gamma \mathcal{R}_{m,m}^{i\kappa}$. Furthermore, in analogy with [AGHH, sec II.1] one expects that a non-normalized one corresponding to a solution ϕ of the above equation is

$$\psi(x) = \int_\Gamma G_{i\kappa}(x-x(s))\phi(s) ds$$

a proof of this claim can be found in the sequel to the paper [Po].

5.4. Application to star graphs

Let us now see what equation (5.4) looks like for graphs of the particular form considered here. Define

$$d_{ij}(s, s') \equiv d_{ij}^\beta(s, s') = \sqrt{s^2 + s'^2 - 2ss' \cos |\vartheta_j - \vartheta_i|} \tag{5.5}$$

with $\vartheta_j - \vartheta_i = \sum_{l=i+1}^j \beta_l$, in particular, $d_{ii}(s, s') = |s - s'|$. By $\mathcal{R}_{ij}^\kappa(\beta) = \mathcal{R}_{ji}^\kappa(\beta)$ we denote the operator $L^2(\mathbb{R}^+) \rightarrow L^2(\mathbb{R}^+)$ with the kernel

$$\mathcal{R}_{ij}^\kappa(s, s'; \beta) := \frac{\gamma}{2\kappa} K_0(\kappa d_{ij}(s, s'))$$

then (5.4) is equivalent to the matrix integral-operator equation

$$\sum_{j=1}^N (\mathcal{R}_{ij}^\kappa(\beta) - \delta_{ij}I) \phi_j = 0 \quad i = 1, \dots, N \tag{5.6}$$

on $\bigoplus_{j=1}^N L^2(\mathbb{R}^+)$. Note that the above kernel has a monotonicity property,

$$\mathcal{R}_{ij}^\kappa(\beta) > \mathcal{R}_{ij}^\kappa(\beta') \tag{5.7}$$

if $|\vartheta_j - \vartheta_i| < |\vartheta'_j - \vartheta'_i|$. This has the following easy consequence:

Proposition 5.12. *Each isolated eigenvalue $\epsilon_n(\beta)$ of $H_2(\beta)$ is an increasing function of β in $(0, \pi)$.*

Proof. Note first that the eigenfunction related to $\epsilon_n(\beta)$ is even with respect to the interchange of the two halflines. Without loss of generality we may assume that $\arg L_j = (-1)^{j-1} \beta/2$. The odd part of $H_2(\beta)$ then corresponds to the Dirichlet condition at $x = 0$. The spectrum of this operator remains the same if we change $\arg L_1$ to $\pi - \beta/2$. Removing then the Dirichlet condition, we get the operator $H_2(\pi)$ with $\inf \sigma(H_2(\pi)) = \inf \sigma_{\text{ess}}(H_2(\beta))$, so by the minimax principle no eigenfunction of $H_2(\beta)$ can be odd.

On the symmetric subspace the diagonal matrix element of the matrix integral operator $\mathcal{R}^\kappa(\beta)$ equals

$$\langle \phi, \mathcal{R}^\kappa(\beta)\phi \rangle = 2\langle \phi_1, \mathcal{R}_{11}^\kappa \phi_1 \rangle + 2\langle \phi_1, \mathcal{R}_{12}^\kappa(\beta)\phi_1 \rangle$$

with the first term on the rhs independent of β . Next we note that $\{\mathcal{R}^\kappa(\beta)\}$ is a type (A) analytic family around any $\beta \in (0, \pi)$; the derivative $\frac{d}{d\beta} \mathcal{R}^\kappa(\beta)$ is a bounded operator or the form $\begin{pmatrix} 0 & \mathcal{D}_\beta \\ \mathcal{D}_\beta & 0 \end{pmatrix}$ where \mathcal{D}_β has the kernel

$$\mathcal{D}_\beta(s, s') = -\frac{\gamma}{2} K_1(\kappa d_{12}^\beta(s, s')) \frac{ss' \sin \beta}{d_{12}^\beta(s, s')} < 0.$$

At the same time $\{\mathcal{R}^\kappa(\beta)\}$ is a type (A) analytic family w.r.t. κ around any $\kappa \in (0, \infty)$ and the corresponding derivative is a bounded operator $\begin{pmatrix} \mathcal{R}'_{11} & \mathcal{R}'_{12} \\ \mathcal{R}'_{12} & \mathcal{R}'_{22} \end{pmatrix}$ with the kernel

$$\mathcal{R}'_{ij}(s, s') = -\frac{\gamma}{2\kappa^2} [K_0(\kappa d_{ij}^\beta(s, s')) + \kappa d_{ij}^\beta(s, s') K_1(\kappa d_{ij}^\beta(s, s'))] < 0.$$

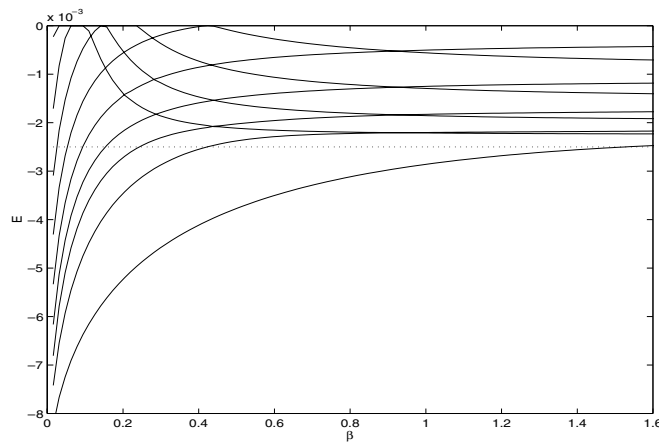


Figure 8. The dependence of the discrete spectrum of $H_{Y,\alpha}$ on the angle β for the symmetric two-arm star Γ_1 . The dotted line represents the threshold $-\gamma^2/4$.

Let $\phi^\beta = \begin{pmatrix} \phi_1^\beta \\ \phi_2^\beta \end{pmatrix}$ be a normalized eigenvector of $\mathcal{R}^\kappa(\beta)$ corresponding to the eigenvalue $\lambda(\kappa, \beta) = \langle \phi^\beta, \mathcal{R}^\kappa(\beta)\phi^\beta \rangle$. By the Feynman–Hellmann theorem we find

$$\frac{d}{d\beta}\lambda(\kappa, \beta) = 2\langle \phi_1^\beta, \mathcal{D}_\beta\phi_1^\beta \rangle < 0$$

and similarly $\frac{d}{d\kappa}\lambda(\kappa, \beta) < 0$. The solution $\kappa = \kappa(\beta)$ of the implicit equation $\lambda(\kappa, \beta) = 1$ thus satisfies

$$\frac{d}{d\beta}\kappa(\beta) = -\frac{d\lambda/d\beta}{d\lambda/d\kappa} < 0$$

and, consequently, the eigenvalue $-\kappa(\beta)^2$ is increasing w.r.t. β . \square

5.5. Numerical results

Having explained analytically how the discrete spectrum of $H_N(\beta)$ depends on the number of arms and the angles β , we employ now the approximation by point-potential Schrödinger operators to obtain the numerical results for cut-off stars which illustrate the above conclusions.

Consider a two-arm star graph Γ_1 with both arms of the same length, $L_1 = L_2 = 300$, and put $\gamma = 0.1$. As we already know, the threshold of the continuous spectrum of $H_2(\beta)$ is $-\gamma^2/4 = -0.0025$. We approximate $H_2(\beta)$ by point-potential Schrödinger operator $H_{Y,\alpha}$ that has one potential at the centre of the star graph and 200 equidistant point potentials on each arm. Only the lower part of the discrete spectrum of $H_{Y,\alpha}$ approximates the discrete spectrum of the star-graph operator, while the upper part corresponds to the interval $[-\gamma^2/4, 0] \subset \sigma_{\text{ess}}(H_2(\beta))$. Therefore, only the states with energy below the threshold may be indeed understood as the approximation of the bound states of $H_2(\beta)$.

The main result of the analytic argument presented above was the dependence of the eigenvalues on the angle β : if β decreases, the eigenvalues decrease and their number grows. The discrete spectrum of $H_{Y,\alpha}$ for β varying is in good agreement with this fact as figure 8 illustrates. The eigenvalue crossings we observe are actual, which is a consequence of the symmetry of the graph Γ_1 . For a non-symmetric graph the crossings become avoided. To demonstrate it in figure 9, we slightly change the length of one arm, $L_2 = 306$, while the other parameters are preserved. Also the setting of the point potentials approximating the new graph Γ_2 stays the same, up to extra four potentials added on the longer arm.

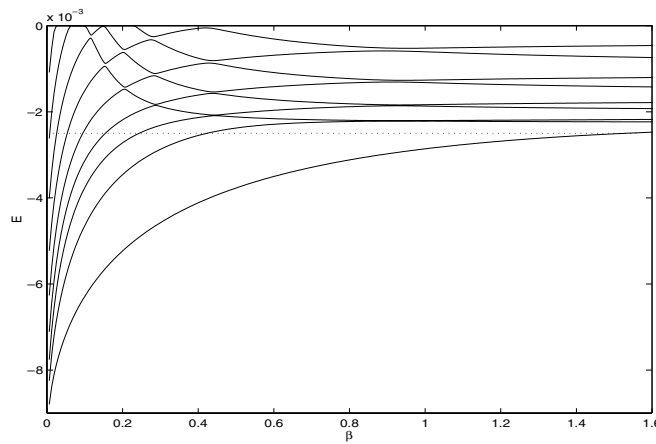


Figure 9. The dependence of the discrete spectrum of $H_{Y,\alpha}$ on the angle β for the non-symmetric two-arm star Γ_2 . The dotted line represents the threshold $-\gamma^2/4$.

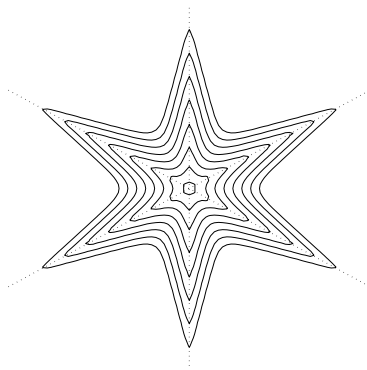


Figure 10. The wavefunction of the ground state of $H_{Y,\alpha}$, $E_0 = -0.612$, which approximates the ground state of $H_6(\beta)$ with β being the 5-tuple of $\pi/3$ and $\gamma = 1$. The contours correspond to logarithmically scaled horizontal cuts, the dotted lines represent the graph Γ .

Expression (4.2) again yields the eigenfunctions in the form of a sum of the free Green functions. We limit ourselves to a pair of examples: the ground state of $H_6(\beta)$ in figure 10 and the third excited state of $H_{10}(\beta)$ in figure 11. The length of the cut arms is 30, in the former case the approximating operator $H_{Y,\alpha}$ has 601 point potentials and in the latter case the number of point potentials is 1001. We see, in particular, that for N large enough $H_N(\beta)$ may have closed nodal lines; it is an interesting question what is the minimal N for which this happens.

6. L^2 -approach to resonances

Our last example, as indicated in the introduction, concerns the situation when Γ is a single infinite curve; we want to see whether resonances in the scattering of states propagating along Γ may be detected by inspecting the spectrum of the cut-off problem with the curve of finite length which is a parameter to be varied.

Consider a curve Γ from figure 12: its central part consists of three segments of a circle with the radius $R = 10$ and it has two infinite ‘legs’. The distance between two closest points

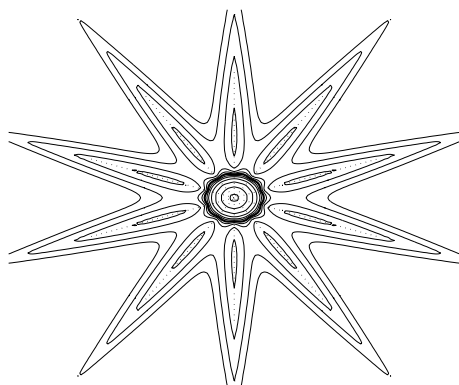


Figure 11. The wavefunction of the third excited state of $H_{Y,\alpha}$, $E_3 = -0.265$. It approximates the third excited state of $H_{10}(\beta)$ with β being the 9-tuple of $\pi/5$ and $\gamma = 1$. The convention is the same as above, the solid line is the nodal line.

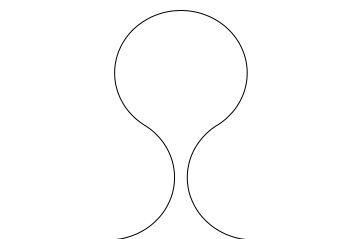


Figure 12. An example of the curve Γ : $R = 10$ and $\Delta = 1.9$.

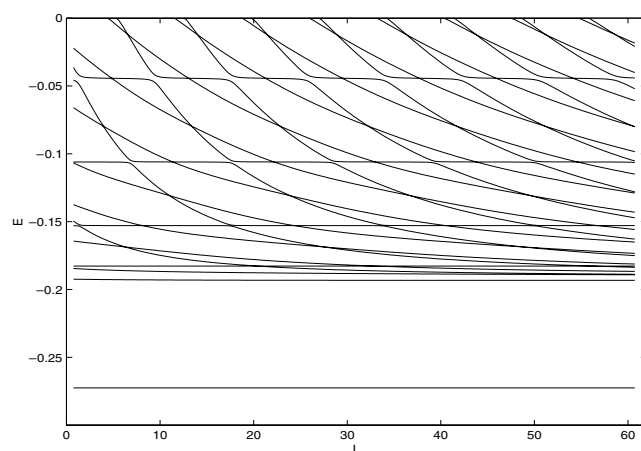


Figure 13. The dependence of the discrete spectrum of the $H_{Y,\alpha}$ on the length L for $R = 10$, $\gamma = 1$ and $\Delta = 1.9$.

of the curve, i.e. the bottleneck width, is denoted by Δ . The coupling constant γ equals 1. We cut the ‘legs’ of the graph to a finite length L and we plot the eigenvalues computed using the approximation for L varying. The number of point potentials involved in $H_{Y,\alpha}$ is chosen so that the distance between every two adjacent points equals 0.3. For small values $\Delta = 1.9$ and $\Delta = 2.9$ the tunnelling effect occurs and we can see the *plateaux* in figures 13, 14, which

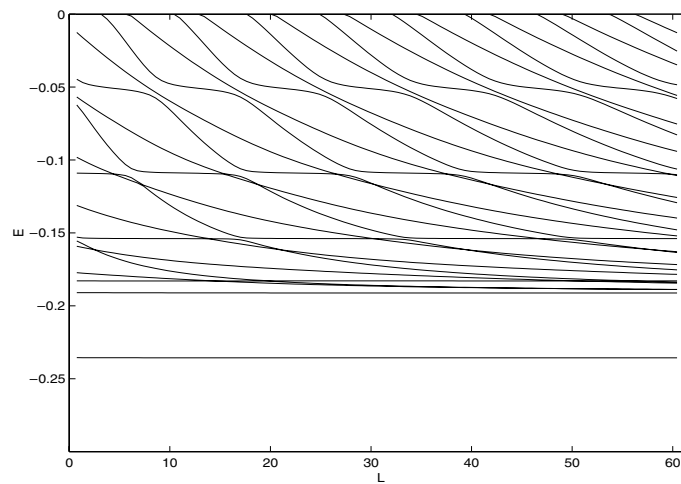


Figure 14. The dependence of the discrete spectrum of $H_{Y,\alpha}$ on the length L for $R = 10$, $\gamma = 1$ and $\Delta = 2.9$.

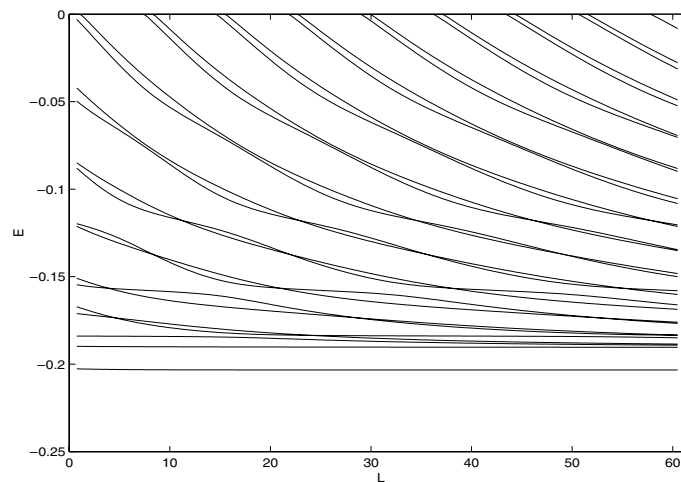


Figure 15. The dependence of the discrete spectrum of $H_{Y,\alpha}$ on the length L for $R = 10$, $\gamma = 1$ and $\Delta = 5.2$.

indicate the existence of resonances; the width of the avoided crossings increases with Δ as expected. On the other hand, for a more open curve, $\Delta = 5.2$, we get a different picture, where the *plateaux* are absent (see figure 15).

The second graph type we are interested in is simple bends, in terms of section 5 it is a two-arm star $\Gamma(\beta)$. As we have already mentioned, avoided eigenvalue crossings are not expected here because the transport along the graph arm involves a single transverse mode—this is confirmed in figure 16, which shows the results of the cut-off method for $\beta = \pi/4$.

Finally to illustrate that resonances may also result from multiple reflections rather than from a tunnelling, we apply the cut-off method to graphs which are of stair-type, or Z-shaped.

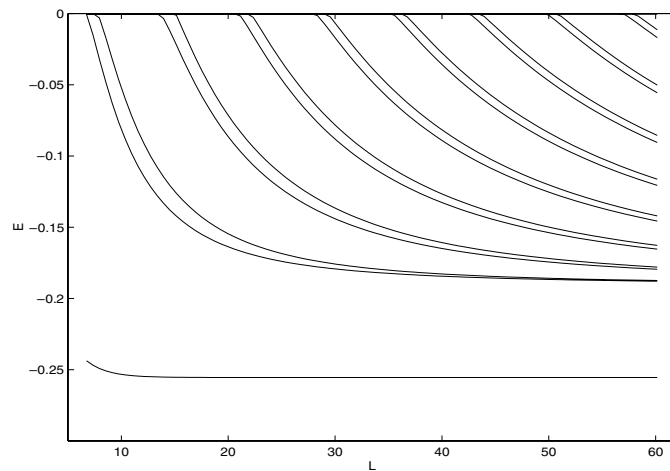


Figure 16. The dependence of the discrete spectrum of $H_{Y,\alpha}$ on the arm length L for the angle $\beta = \pi/4$ and $\gamma = 1$.

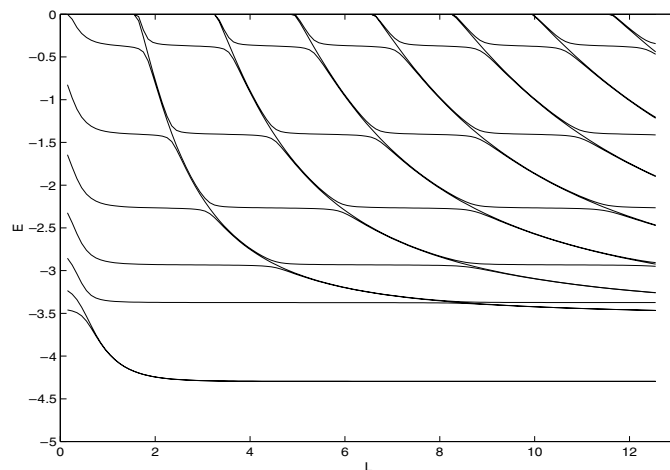


Figure 17. The dependence of the discrete spectrum of $H_{Y,\alpha}$ on the arm length L for $R = 10$, $\theta = 0.32\pi$ and $\gamma = 5$.

They consist of three line segments: the central one has a finite length R , i.e. the ‘height’ of the stair, the other two are parallel (cut-off) halflines. If the angle θ between the segments is less than $\pi/2$ the term Z-shaped is more appropriate. The results for $R = 10$ and $\gamma = 5$ are plotted in figures 17 and 18. In the former case the stair is ‘skewed’ to $\theta = 0.32\pi$, in the latter we have $\theta = \pi/2$; the distance between the point potentials of the approximating operator $H_{Y,\alpha}$ equals 0.1. We find avoided crossings, however, they are very narrow for $\theta = 0.32\pi$ and barely visible in the right-angle case; this observation can be naturally understood in terms of the reflection probability through a single bend—compare with the angle dependence of the spectrum in figure 8.

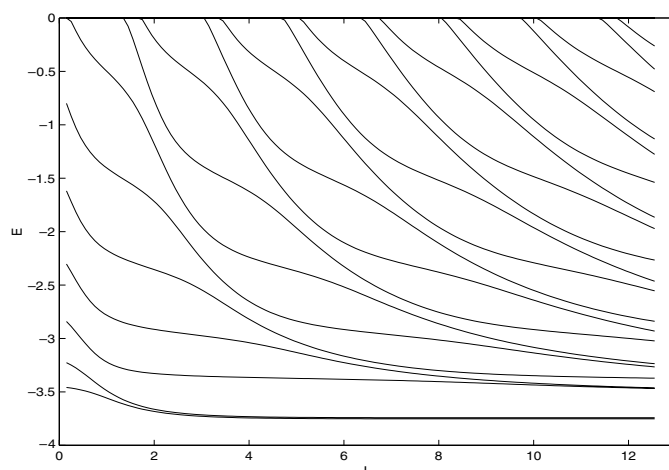


Figure 18. The dependence of the discrete spectrum of $H_{Y,\alpha}$ on the arm length L for $R = 10$, $\theta = \pi/2$ and $\gamma = 5$.

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