On the spectrum of a bent chain graph

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Abstract

We study Schrödinger operators on an infinite quantum graph of a chain form which consists of identical rings connected at the touching points by δ-couplings with a parameter $\alpha \in \mathbb{R}$. If the graph is "straight", i.e. periodic with respect to ring shifts, its Hamiltonian has a band spectrum with all the gaps open whenever $\alpha \neq 0$. We consider a "bending" deformation of the chain consisting of changing one position at a single ring and show that it gives rise to eigenvalues in the open spectral gaps. We analyze dependence of these eigenvalues on the coupling α and the "bending angle" as well as resonances of the system coming from the bending. We also discuss the behaviour of the eigenvalues and resonances at the edges of the spectral bands.

1 Introduction

Quantum graphs, i.e. Schrödinger operators with graph configuration spaces, were introduced in the middle of the last century [RuS53] and rediscovered three decades later [GP88, EŠ89]. Since then they attracted a lot of attention; they became both a useful tool in numerous applications and a mean which makes easy to study fundamental properties such as quantum chaos. We refrain from giving an extensive bibliography and refer to the recent proceedings volume [AGA] which the reader can use to check the state of art in this area.

One of the frequent questions concerns relations between the geometry of a graph Γ and spectral properties of a Schrödinger operator supported by Γ. Put like that, the question allows different interpretation. On one hand, we can have in mind the intrinsic geometry of Γ which enters the problem through the adjacency matrix of the graph and the lengths of its edges. On the other hand, quite often one thinks of Γ as of a subset of $\mathbb{R}^n$ with the geometry inherited from the ambient space. In that case geometric perturbations can acquire a

rather illustrative meaning and one can ask in which way they influence spectral properties of a quantum particle "living" on Γ; in this context one can think of graphs which are "bent", locally "protruded" or "squeezed", etc.

The aim of the present paper is to analyze the influence of a "bending" deformation on a graph which exhibits a one-dimensional periodicity. Without striving for generality we will discuss in detail a simple nontrivial example in which the unperturbed system is a "chain graph" consisting of an array of rings of unit radius, cf. Fig. 1, connected through their touching points. We suppose
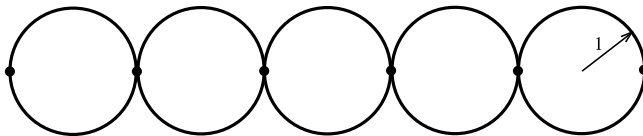

Figure 1: The unperturbed chain graph

that there are no external fields. Since values of physical constants are not important in our considerations we put $\hbar = 2m = 1$ and identify the particle Hamiltonian with the (negative) Laplacian acting as $\psi_j \mapsto -\psi_j''$ on each edge of the graph. It is well known that in order to get a self-adjoint operator one has to impose appropriate boundary conditions at the graph vertices. In our model we employ the so-called δ-coupling characterized by the conditions

$$\psi_j(0) = \psi_k(0) =: \psi(0)\,, \quad j,k \in \hat{n}\,, \qquad \sum_{j=1}^{n} \psi_j'(0) = \alpha\psi(0)\,, \qquad (1.1)$$

where $\hat{n} = \{1, 2, \dots, n\}$ is the index set numbering the edges emanating from the vertex — in our case $n = 4$ — and $\alpha \in \mathbb{R} \cup \{+\infty\}$ is the coupling constant supposed to be the same at every vertex of the chain. It is important that the "straight" graph has spectral gaps, thus we *exclude the free boundary conditions* (sometimes called, not quite appropriately, Kirchhoff), i.e. we assume $\alpha \neq 0$.

The geometric perturbation to consider is the simplest possible bending of such a chain obtained by a shift of one of the contact points, as sketched in Fig. 2, which is parametrized by the bending angle ϑ characterizing the ratio of the two edges constituting the perturbed ring. Our aim is to show that the bending gives rise to eigenvalues in the gaps of the unperturbed spectrum and to analyze how they depend on ϑ. At the same time the bent chain will exhibit resonances and we will discuss behaviour of the corresponding poles.

The contents of the paper is the following. In the next section we analyze the straight chain. Using Bloch-Floquet decomposition we will show that the spectrum consists of infinite number of absolutely continuous spectral bands separated by open gaps, plus a family of infinitely degenerate eigenvalues at
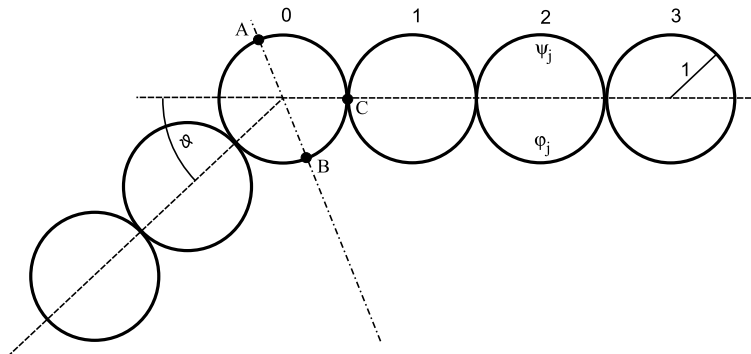
Figure 2: A bent graph

band edges. In Section 3 we will analyze the discrete spectrum due to the bend-
ing showing that in each gap it gives rise to at most two eigenvalues. Section 4
describes their dependence on the bending angle as well as complex solutions
to the spectral condition corresponding to resonances in the bent chain. In
Section 5 we discuss further the angular dependence with attention to singular
points where the solutions coincide with the band edges. Finally, in the con-
cluding remarks we draw a parallel of our results with properties of quantum
waveguides.

2   An infinite periodic chain

First we consider a "straight" chain Γ_0 as sketched in Fig. 1; without loss of
generality we may suppose that the circumference of each ring is 2π. The state
Hilbert space of a nonrelativistic and spinless particle living on Γ_0 is $L^2(\Gamma_0)$. We
suppose that the particle is free, not interacting with an external potentials on
the edges, and denote by H_0 its Hamiltonian, i.e. it acts as the negative Lapla-
cian on each graph link and its domain consists of all functions from $W_{\mathrm{loc}}^{2,2}(\Gamma_0)$
which satisfy the δ boundary conditions (1.1) at the vertices of Γ_0; we suppose
that the coupling constant α is the same at each vertex[1].

In view of the periodicity of Γ_0, the spectrum of H_0 can be computed us-
ing Bloch-Floquet decomposition. Let us consider an elementary cell with the
wavefunction components denoted according to the Fig. 3 and ask about the
spectrum of the Floquet components of H_0. Since the operator acts as a negative
second derivative, each component of the eigenfunction with energy $E = k^2 \neq 0$
is a linear combination of the functions $\mathrm{e}^{\pm ikx}$. The momentum k is convention-
ally chosen positive for $E > 0$, while for E negative we put $k = i\kappa$ with $\kappa > 0$

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[1]The coupling constant α is kept fixed and for the sake of simplicity we will not use it to
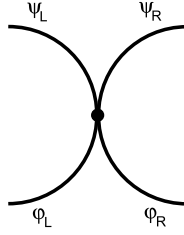label the Hamiltonian neither in the straight nor in the bent case.

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Figure 3: Elementary cell of the periodic system

(the case $E = 0$ will be mentioned separately below). For a given $E \neq 0$, the wavefunction components on the elementary cell are therefore given by

$$
\begin{aligned}
\psi_L(x) &= C_L^+ \mathrm{e}^{\mathrm{i}kx} + C_L^- \mathrm{e}^{-\mathrm{i}kx}, && x \in [-\pi/2, 0] \\
\psi_R(x) &= C_R^+ \mathrm{e}^{\mathrm{i}kx} + C_R^- \mathrm{e}^{-\mathrm{i}kx}, && x \in [0, \pi/2] \\
\varphi_L(x) &= D_L^+ \mathrm{e}^{\mathrm{i}kx} + D_L^- \mathrm{e}^{-\mathrm{i}kx}, && x \in [-\pi/2, 0] \\
\varphi_R(x) &= D_R^+ \mathrm{e}^{\mathrm{i}kx} + D_R^- \mathrm{e}^{-\mathrm{i}kx}, && x \in [0, \pi/2]
\end{aligned}
\tag{2.1}
$$

As we have said, at the contact point the δ-coupling (1.1) is assumed, i.e.

$$
\psi_L(0) = \psi_R(0) = \varphi_L(0) = \varphi_R(0)
$$
$$
-\psi_L'(0) + \psi_R'(0) - \varphi_L'(0) + \varphi_R'(0) = \alpha \cdot \psi_L(0)
\tag{2.2}
$$

On the other hand, at the "free" ends of the cell the Floquet conditions are imposed,

$$
\begin{aligned}
\psi_R(\pi/2) &= \mathrm{e}^{\mathrm{i}\theta} \psi_L(-\pi/2) & \psi_R'(\pi/2) &= \mathrm{e}^{\mathrm{i}\theta} \psi_L'(-\pi/2) \\
\varphi_R(\pi/2) &= \mathrm{e}^{\mathrm{i}\theta} \varphi_L(-\pi/2) & \varphi_R'(\pi/2) &= \mathrm{e}^{\mathrm{i}\theta} \varphi_L'(-\pi/2)
\end{aligned}
\tag{2.3}
$$

with θ running through $[-\pi, \pi)$; alternatively we may say that the quasimomentum $\frac{1}{2\pi}\theta$ runs through $[-1/2, 1/2)$, the Brillouin zone of the problem.

Substituting (2.1) into (2.2) and (2.3), one obtains after simple manipulations

$$
C_X^+ \cdot \sin k\pi = D_X^+ \cdot \sin k\pi, \quad C_X^- \cdot \sin k\pi = D_X^- \cdot \sin k\pi,
\tag{2.4}
$$

where X stands for L or R, hence $C_X^+ = C_X^-$ and $D_X^+ = D_X^-$ provided $k \notin \mathbb{N}_0 := \{0, 1, 2, \dots\}$. We will treat the special case $k \in \mathbb{N}$ later, now we will suppose k does not belong to $\mathbb{N}$, the set of natural numbers. Furthermore, from (2.2) and (2.3) we obtain an equation for the phase factor $\mathrm{e}^{\mathrm{i}\theta}$,

$$
\mathrm{e}^{2\mathrm{i}\theta} - \mathrm{e}^{\mathrm{i}\theta} \left(2\cos k\pi + \frac{\alpha}{2k} \sin k\pi \right) + 1 = 0,
\tag{2.5}
$$

which has real coefficients for any $k \in \mathbb{R} \cup \mathrm{i}\mathbb{R} \backslash \{0\}$ and the discriminant equal to

$$
D = \left(2\cos k\pi + \frac{\alpha}{2k} \sin k\pi \right)^2 - 4.
$$

We have to determine values of k^2 for which there is a $\theta \in [-\pi, \pi)$ such that (2.5) is satisfied, in other words, for which k^2 it has, as an equation in the unknown $e^{i\theta}$, at least one root of modulus one. Note that a pair of solutions of (2.5) always give one when multiplied, regardless the value of k, hence either both roots are complex conjugated of modulus one, or one is of modulus greater than one and the other has modulus smaller than one. Obviously, the latter situation corresponds to a positive discriminant, and the former one to the discriminant less or equal to zero. We summarize this discussion as follows:

Proposition 2.1. *If $k^2 \in \mathbb{R}\backslash\{0\}$ and $k \notin \mathbb{N}$, then $k^2 \in \sigma(H_0)$ if and only if the condition*

$$\left| \cos k\pi + \frac{\alpha}{4} \cdot \frac{\sin k\pi}{k} \right| \leq 1 \tag{2.6}$$

is satisfied.

In particular, the negative spectrum is obtained by putting $k = i\kappa$ for $\kappa > 0$ and rewriting the inequality (2.6) in terms of this variable. Note that since $\sinh x \neq 0$ for all $x > 0$, it never occurs that $\sin k\pi = 0$ for $k \in i\mathbb{R}^+$, the positive imaginary axis, thus there is no need to treat this case separately like for $k \in \mathbb{R}^+$, cf. (2.4) above.

Corollary 2.2. *If $\kappa > 0$, then $-\kappa^2 \in \sigma(H_0)$ if and only if*

$$\left| \cosh \kappa\pi + \frac{\alpha}{4} \cdot \frac{\sinh \kappa\pi}{\kappa} \right| \leq 1 \,. \tag{2.7}$$

Let us finally mention the case $k \in \mathbb{N}$ left out above. It is straightforward to check that k^2 is then an eigenvalue, and moreover, that it has an infinite multiplicity. One can construct an eigenfunction which is supported by a single circle, which is given by $\psi(x) = \sin kx$ with $x \in [0, \pi]$ on the upper semicircle and $\varphi(x) = -\sin kx$ with $x \in [0, \pi]$ on the lower one.

Remark 2.3. The condition (2.6) reminds us of the corresponding condition in the Kronig-Penney model with the distance between the interaction sites equal to π, cf. [AGHH], the only difference being that the coupling constant is halved, $\frac{1}{2}\alpha$ instead of α. In contrast to that, the point spectrum of the KP model is empty. These facts are easy to understand if we realize that our model has the up-down mirror symmetry, and thus H_0 decomposes into a symmetric and antisymmetric part. The former is unitarily equivalent to the KP model with modified coupling, the latter corresponds to functions vanishing at the vertices, having thus a pure point spectrum. Looking ahead, we remark that the bending perturbation breaks this mirror symmetry.

Finally, in the case $E = 0$ we get in the similar way the equation

$$e^{2i\theta} - e^{i\theta}\left(2 + \frac{\alpha\pi}{2}\right) + 1 = 0 \,, \tag{2.8}$$

replacing (2.5), whence we infer that $0 \in \sigma(H_0)$ if and only if

$$\left| 1 + \frac{\alpha\pi}{4} \right| \leq 1 \,, \tag{2.9}$$

hence zero can belong to the continuous part of the spectrum only and it happens *iff* $\alpha \in [-8/\pi, 0]$. In conclusion, we can make the following claim about $\sigma(H_0)$.

Theorem 2.4. *The spectrum of H_0 consists of infinitely degenerate eigenvalues equal to n^2 with $n \in \mathbb{N}$, and absolutely continuous spectral bands with the following properties:*

If $\alpha > 0$, then every spectral band is contained in an interval $(n^2, (n+1)^2]$ with $n \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$, and its upper edge coincides with the value $(n+1)^2$.

If $\alpha < 0$, then in each interval $[n^2, (n+1)^2)$ with $n \in \mathbb{N}$ there is exactly one spectral band the lower edge of which coincides with n^2. In addition, there is a spectral band with the lower edge (being the overall spectral threshold) equal to $-\kappa^2$, where κ is the largest solution of

$$\left| \cosh \kappa\pi + \frac{\alpha}{4} \cdot \frac{\sinh \kappa\pi}{\kappa} \right| = 1 . \tag{2.10}$$

The position of the upper edge of this band depends on α. If $-8/\pi < \alpha < 0$, then it is equal to k^2 where k is the solution of

$$\cos k\pi + \frac{\alpha}{4} \cdot \frac{\sin k\pi}{k} = -1$$

contained in $(0,1)$. On the other hand, for $\alpha < -8/\pi$ the upper edge is negative, $-\kappa^2$ with κ being the smallest solution of (2.10), and for $\alpha = -8/\pi$ it equals zero.

Finally, $\sigma(H_0) = [0, +\infty)$ holds if $\alpha = 0$.

Proof. The degenerate bands, in other words, the eigenvalues of infinite multiplicity, were found already and it is straightforward to check that no other eigenvalues exist. The continuous spectrum can be in view of Remark 2.3 treated as in [AGHH], nevertheless, we sketch the argument not only to make the paper self-contained, but also in view of next sections where some ideas and formula of the present proof will be used again.

Consider first the positive part of the continuous spectrum. The condition (2.6) clearly determines bands with one endpoint at n^2, $n \in \mathbb{N}$, where the sign of α decides whether it is the upper or lower one. If $\alpha < 0$, the presence of a band in (0,1) depends on $|\alpha|$. Denoting $g(x) := \cos x\pi + \frac{\alpha}{4} \cdot \frac{\sin x\pi}{x}$ we want to show that $B := \{x \in (0,1) : |g(x)| \le 1\}$ is either empty or an interval with zero as its edge. It is obvious that g maps $(0,1)$ continuously into $(-\infty, 1)$; we will check that $g(x_0) = -1$ implies $g'(x_0) < 0$. We notice first that the premise implies $\cos x_0\pi = -1 - \frac{\alpha}{4} \cdot \frac{\sin x_0\pi}{x_0}$; taking the square of this relation we find after simple manipulations that $\sin x_0\pi = -2 \left(\frac{\alpha}{4x_0} + \frac{4x_0}{\alpha} \right)^{-1}$ and $\cos x_0\pi = \left(\frac{\alpha}{4x_0} - \frac{4x_0}{\alpha} \right) \left(\frac{\alpha}{4x_0} + \frac{4x_0}{\alpha} \right)^{-1}$. Evaluating $g'(x_0)$ and substituting these expressions we get

$$g'(x_0) = \frac{\alpha\pi}{4x_0} \left(1 - \frac{\sin \pi x_0}{\pi x_0} \right) < 0 .$$

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These properties together with the continuity of g imply that if B is not empty, then it is an interval with the left endpoint zero. It is also clear that B is non-empty *iff* $g(0+) > -1$ which gives the condition $\alpha > -8/\pi$. On the contrary, B is empty if $\alpha < -8/\pi$ and the borderline case $\alpha = -8/\pi$ was mentioned above.

Let us next focus on the negative part using $\tilde{g}(x) := \cosh x\pi + \frac{\alpha}{4} \cdot \frac{\sinh x\pi}{x}$ and ask about $\tilde{B} := \{x \in (0, \infty) : |\tilde{g}(x)| \leq 1\}$. It is easy to check that $\tilde{g}(x) = -1$ iff $\tanh \frac{x\pi}{2} = \frac{4x}{|\alpha|}$ and $\tilde{g}(x) = 1$ iff $\coth \frac{x\pi}{2} = \frac{4x}{|\alpha|}$. It implies that there is exactly one x_1 such that $\tilde{g}(x_1) = 1$, and that the equation $\tilde{g}(x) = -1$ has one solution x_{-1} in the case $\alpha < -8/\pi$ and no solution in the case $\alpha \in [-8/\pi, 0)$. Since obviously $0 < x_{-1} < x_1$ and $\tilde{g}(0+) := \lim_{x \to 0_+} \tilde{g}(x) = 1 + \alpha\pi/4$, we infer that $\tilde{B}$ is a bounded interval. Its closure contains zero *iff* $\alpha \in [-8/\pi, 0)$ because then $\tilde{g}(0+) \in [-1, 1)$. In such a case the lowest spectral band is the closure of $B \cup \tilde{B}$, otherwise it is the closure of $\tilde{B}$ only. $\qquad\square$

3 The perturbed system

3.1 General considerations

Let us suppose now that the straight chain of the previous section suffers a bending perturbation as shown in Figure 2. We call the perturbed graph Γ_ϑ; it differs from Γ_0 by replacing the arc lengths π of a fixed ring, conventionally numbered as zero, by $\pi \pm \vartheta$. The bending angle ϑ is supposed to take values from $(0, \pi)$, regardless of the fact that for $\vartheta \geq 2\pi/3$ it is not possible to consider Γ_ϑ as embedded in the plane as sketched — one can certainly realize such a "bending" in an alternative way, for instance, by deforming the selected ring.

The state Hilbert space of the perturbed system is $L^2(\Gamma_\vartheta)$ and the Hamiltonian is H_ϑ obtained by a natural modification of H_0; our aim is to determine its spectrum. Since Γ_ϑ has the mirror symmetry w.r.t. the axis of the zeroth ring passing through the points $x = \frac{1}{2}(\pi \pm \vartheta)$, the operator H_ϑ can be reduced by parity subspaces into a direct sum of an even part, H^+, and odd one, H^-; for the sake of simplicity we drop mostly the subscript ϑ in the following.

All the components of the wavefunction at energy k^2 are linear combinations of $e^{\pm ikx}$. As we have said we use the ring labelling with zero corresponding to the perturbed one; the mirror symmetry allows us to study a half of the system only, say, with non-negative indices. The wavefunction on each ring will be a pair of functions ψ_j and φ_j, where j is the circle index, ψ_j corresponds to the upper semicircle and φ_j to the lower one,

$$
\begin{aligned}
\psi_j(x) &= C_j^+ e^{ikx} + C_j^- e^{-ikx}, \quad x \in [0, \pi], \\
\varphi_j(x) &= D_j^+ e^{ikx} + D_j^- e^{-ikx}, \quad x \in [0, \pi]
\end{aligned}
\tag{3.1}
$$

for $j \in \mathbb{N}$. The situation is different in the case $j = 0$, where the variables run

over modified intervals,

$$\psi_0(x) = C_0^+ \mathrm{e}^{\mathrm{i}kx} + C_0^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in \left[\frac{\pi - \vartheta}{2}, \pi\right]$$
$$\varphi_0(x) = D_0^+ \mathrm{e}^{\mathrm{i}kx} + D_0^- \mathrm{e}^{-\mathrm{i}kx}, \quad x \in \left[\frac{\pi + \vartheta}{2}, \pi\right]$$

$$(3.2)$$

There are δ-couplings with the parameter α in the points of contact, i.e.

$$\psi_j(0) = \varphi_j(0) \qquad \psi_j(\pi) = \varphi_j(\pi) \tag{3.3}$$

and

$$\psi_j(0) = \psi_{j-1}(\pi) \tag{3.4}$$
$$\psi_j'(0) + \varphi_j'(0) - \psi_{j-1}'(\pi) - \varphi_{j-1}'(\pi) = \alpha \cdot \psi_j(0) \tag{3.5}$$

Substituting (3.1) into (3.3) we obtain

$$C_j^+ \cdot \sin k\pi = D_j^+ \cdot \sin k\pi \quad \text{and} \quad C_j^- \cdot \sin k\pi = D_j^- \cdot \sin k\pi \,,$$

thus for $k \notin \mathbb{N}_0$ we have $C_j^+ = D_j^+$ and $C_j^- = D_j^-$. The case $k \in \mathbb{N}_0$ can be treated in analogy analogously with the "straight" case: it is easy to see that squares of integers are infinitely degenerate eigenvalues and the eigenfunctions can be supported by any ring, now with the exception of the zeroth one. From now on, we suppose $k \notin \mathbb{N}_0$.

Using the coupling conditions (3.4) and (3.5), we arrive at a "transfer matrix" relation between coefficients of the neighbouring rings,

$$\begin{pmatrix} C_j^+ \\ C_j^- \end{pmatrix} = \underbrace{\begin{pmatrix} \left(1 + \frac{\alpha}{4\mathrm{i}k}\right) \mathrm{e}^{\mathrm{i}k\pi} & \frac{\alpha}{4\mathrm{i}k} \mathrm{e}^{-\mathrm{i}k\pi} \\ -\frac{\alpha}{4\mathrm{i}k} \mathrm{e}^{\mathrm{i}k\pi} & \left(1 - \frac{\alpha}{4\mathrm{i}k}\right) \mathrm{e}^{-\mathrm{i}k\pi} \end{pmatrix}}_{M} \cdot \begin{pmatrix} C_{j-1}^+ \\ C_{j-1}^- \end{pmatrix}, \tag{3.6}$$

valid for all $j \geq 2$, which yields

$$\begin{pmatrix} C_j^+ \\ C_j^- \end{pmatrix} = M^{j-1} \cdot \begin{pmatrix} C_1^+ \\ C_1^- \end{pmatrix}. \tag{3.7}$$

It is clear that the asymptotical behavior of the norms of $(C_j^+, C_j^-)^T$ is determined by spectral properties of the matrix M. Specifically, let $(C_1^+, C_1^-)^T$ be an eigenvector of M corresponding to an eigenvalue μ, then $|\mu| < 1$ ($|\mu| > 1$, $|\mu| = 1$) means that $\|(C_j^+, C_j^-)^T\|$ decays exponentially with respect to j (respectively, it is exponentially growing, or independent of j).

The wavefunction components on the j-th ring for both $H^\pm$ (as well as on the $(-j)$-th by the mirror symmetry) are determined by C_j^+ and C_j^-, and thus by $(C_1^+, C_1^-)^T$ by virtue of (3.7). If $(C_1^+, C_1^-)^T$ has a non-vanishing component related to an eigenvalue of M of modulus larger than one, it determines neither an eigenfunction nor a generalized eigenfunction of $H^\pm$. On the other hand,

if $(C_1^+, C_1^-)^T$ is an eigenvector, or a linear combination of eigenvectors, of the matrix M with modulus less than one (respectively, equal to one), then the coefficients $C_j^\pm$ determine an eigenfunction (respectively, a generalized eigenfunction) and the corresponding energy E belongs to the point (respectively, continuous) spectrum of the operator $H^\pm$. To perform the spectral analysis of M, we employ its characteristic polynomial at energy k^2,

$$\lambda^2 - 2\lambda \left(\cos k\pi + \frac{\alpha}{4k} \sin k\pi \right) + 1 \,, \tag{3.8}$$

which we have encountered already in the relation (2.5); it shows that M has an eigenvalue of modulus less than one *iff* the discriminant of (3.8) is positive, i.e.

$$\left| \cos k\pi + \frac{\alpha}{4k} \sin k\pi \right| > 1 \,,$$

and a pair of complex conjugated eigenvalues of modulus one *iff* the above quantity is ≤ 1. In the former case the eigenvalues of M are given by

$$\lambda_{\frac{1}{2}} = \cos k\pi + \frac{\alpha}{4k} \sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k} \sin k\pi \right)^2 - 1} \,,$$

satisfying $\lambda_2 = \lambda_1^{-1}$, hence $\lambda_2 < 1$ holds if $\cos k\pi + \frac{\alpha}{4k} \sin k\pi > 1$ and $\lambda_1 < 1$ if this quantity is < -1. Moreover, the corresponding eigenvectors of M are

$$v_{1,2} = \begin{pmatrix} \frac{\alpha}{4ik} \mathrm{e}^{-ik\pi} \\ \lambda_{1,2} - \left(1 + \frac{\alpha}{4ik} \right) \mathrm{e}^{ik\pi} \end{pmatrix} \,.$$

Remark 3.1. Comparing to (2.6) we see that the perturbation does not affect the spectral bands, and also, that new eigenvalues coming from the perturbation can appear only in the gaps. These facts are obvious, of course, from general principles. Using the natural identification of $L^2(\Gamma_0)$ and $L^2(\Gamma_\vartheta)$ we see that H_0 and H_ϑ differ by a shift of the point where a boundary condition is applied, hence their resolvent difference has a finite rank (in fact, rank two). Consequently, their essential spectra coincide and each spectral gap of H_0 contains at most two eigenvalues of H_ϑ, see [We, Sec. 8.3, Cor. 1].

3.2 Spectrum of H^+

The operator H^+ corresponds to the wave functions *even* w.r.t. the symmetry axis, hence we may consider a half of the graph with the Neumann conditions at the boundary (i.e., the points A, B in Figure 2),

$$\psi_0' \left(\frac{\pi - \vartheta}{2} \right) = 0 \,, \quad \varphi_0' \left(\frac{\pi + \vartheta}{2} \right) = 0 \,.$$

At the contact point of the zeroth and the first ring (denoted by C) there is a δ-coupling with the parameter α,

$$\psi_0(\pi) = \varphi_0(\pi) = \psi_1(0) \tag{3.9}$$
$$\psi_1'(0) + \varphi_1'(0) - \psi_0'(\pi) - \varphi_0'(\pi) = \alpha \cdot \psi_0(\pi) \tag{3.10}$$

Substituting to these conditions from (3.1) and (3.2) and using the equality $\varphi_1'(0) = \psi_1'(0)$, we obtain $(C_1^+, C_1^-)^T$ up to a multiplicative constant,

$$\begin{pmatrix} C_1^+ \\ C_1^- \end{pmatrix} = \begin{pmatrix} \frac{\cos k\pi + \cos k\vartheta}{\sin k\pi} + \mathrm{i}\left(1 - \frac{\alpha(\cos k\pi + \cos k\vartheta)}{2k\sin k\pi}\right) \\ \frac{\cos k\pi + \cos k\vartheta}{\sin k\pi} - \mathrm{i}\left(1 - \frac{\alpha(\cos k\pi + \cos k\vartheta)}{2k\sin k\pi}\right) \end{pmatrix}.$$

The right-hand side is well defined except for $\sin k\pi = 0$, but this case has been already excluded from our considerations; we know that for $k \in \mathbb{N}$ the number k^2 is an eigenvalue of infinite multiplicity.

Following the above discussion $k^2 \in \sigma_p(H^+)$ requires that the vector $(C_1^+, C_1^-)^T$ is an eigenvector of M corresponding to the eigenvalue λ of the modulus less than one. Using the above explicit form of the eigenvectors and solving the equation

$$\begin{vmatrix} \frac{\cos k\pi + \cos k\vartheta}{\sin k\pi} + \mathrm{i}\left(1 - \frac{\alpha(\cos k\pi + \cos k\vartheta)}{2k\sin k\pi}\right) & \frac{\alpha}{4ik}\mathrm{e}^{-ik\pi} \\ \frac{\cos k\pi + \cos k\vartheta}{\sin k\pi} - \mathrm{i}\left(1 - \frac{\alpha(\cos k\pi + \cos k\vartheta)}{2k\sin k\pi}\right) & \lambda - \left(1 + \frac{\alpha}{4ik}\right)\mathrm{e}^{ik\pi} \end{vmatrix} = 0$$

we arrive at the condition

$$(\cos k\vartheta + \cos k\pi) \cdot \left(\frac{\alpha}{4k}\sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right)^2 - 1}\right) = \sin^2 k\pi,$$

with the sign given by the sign of $\cos k\pi + \frac{\alpha}{4k}\sin k\pi$. Since $\sin k\pi \neq 0$, the second factor at the *lhs* is also nonzero and the last equation is equivalent to

$$\cos k\vartheta = -\cos k\pi + \frac{\sin^2 k\pi}{\frac{\alpha}{4k}\sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k}\sin k\pi\right)^2 - 1}}; \qquad (3.11)$$

for the sake of brevity we denote the expression at the *rhs* by $f(k)$.

The relation (3.11) is our main tool to analyze the discrete spectrum and we are going to discuss now its solutions. We start with an auxiliary result noting that, as a consequence of Theorem 2.4, the set of positive k for which the inequality $|\cos k\pi + \frac{\alpha}{4k}\sin k\pi| \geq 1$ is satisfied is an infinite disjoint union of closed intervals. We denote them I_n with $n \in \mathbb{N}$ and recall that $n \in I_n$. If $\alpha > 0$ we denote by I_0 the interval with the edge at zero corresponding to the non-negative part of the lowest spectral gap of H_0.

Proposition 3.2. *The function f introduced above maps each $I_n \backslash \{n\}$ into the interval $(-1, 1) \cup \{(-1)^n\}$. Moreover, $f(x) = (-1)^n$ holds for $x \in I_n \backslash \{n\}$ iff $|\cos x\pi + \frac{\alpha}{4x}\sin x\pi| = 1$, and $\lim_{x \in I_n, x \to n} f(x) = (-1)^{n+1}$.*

Proof. According to (3.11), the function f is continuous in each interval $I_n \backslash \{n\}$, thus it maps the interval $I_n \backslash \{n\}$ again to an interval. The claim then follows from the following easy observations. First, $f(x) = (-1)^n$ *iff* x is the non-integer boundary point of I_n (if $\alpha < 0$ and $|\alpha|$ is sufficiently large, the left edge of I_1 is moved to zero and one checks that $\lim_{x \to 0} f(x) = -1$). Furthermore, for all $x \in I_n \backslash \{n\}$ we have $f(x) \neq (-1)^{n-1}$, and finally, $\lim_{x \to n, x \in I_n} f(x) = (-1)^{n-1}$. $\square$

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Proposition 3.2 guarantees the existence of at least one solution of (3.11) in each interval $I_n \backslash \{n\}$, except for the case when ϑ satisfies $\cos n\vartheta = (-1)^{n-1}$, or equivalently, except for the angles $\vartheta = \frac{n+1-2\ell}{n}\pi$, $\ell = 1, \ldots, \left[\frac{n+1}{2}\right]$. Later we will show that for these angles there is indeed no solution of the equation (3.11) in $I_n \backslash \{n\}$, while for the other angles in $(0, \pi)$ there is exactly one.

In a similar way one can proceed with the negative part of the spectrum. If $k = i\kappa$ where $\kappa > 0$, the condition (3.11) acquires the form

$$\cosh \kappa\vartheta = -\cosh \kappa\pi - \frac{\sinh^2 \kappa\pi}{\frac{\alpha}{4\kappa}\sinh \kappa\pi \pm \sqrt{\left(\cosh \kappa\pi + \frac{\alpha}{4\kappa}\sinh \kappa\pi\right)^2 - 1}}, \quad (3.12)$$

where the upper sign in the denominator refers to $\cosh \kappa\pi + \frac{\alpha}{4\kappa}\sinh \kappa\pi > 1$, and the lower one to $\cosh \kappa\pi + \frac{\alpha}{4\kappa}\sinh \kappa\pi < -1$. Let us denote the *rhs* of (3.12) by $\tilde{f}(\kappa)$, then we have the following counterpart to Proposition 3.2.

Proposition 3.3. *If $\alpha \geq 0$, then $\tilde{f}(\kappa) < -\cosh \kappa\vartheta$ holds for all $\kappa > 0$ and $\vartheta \in (0, \pi)$. On the other hand, for $\alpha < 0$ we have*

If $\lim_{\kappa \to 0} \left(\cosh \kappa\pi + \frac{\alpha}{4\kappa}\sinh \kappa\pi\right) < -1$, then there is a right neighbourhood of zero where $\tilde{f}(x) = -1 - C(\alpha)x^2 + o(x^2)$ with the constant explicitly given by $C(\alpha) := \left(\frac{1}{2} + \left(\frac{\alpha\pi}{4} + \sqrt{\left(\frac{\alpha\pi}{4}\right)^2 + \frac{\alpha\pi}{2}}\right)^{-1}\right)\pi^2$. Moreover, $\tilde{f}(\kappa) = -1$ holds for $\kappa > 0$ iff $\cosh \kappa\pi + \frac{\alpha}{4\kappa}\sinh \kappa\pi = -1$.

The interval $\left\{\kappa : \cosh \kappa\pi + \frac{\alpha}{4\kappa}\sinh \kappa\pi \geq 1 \wedge \kappa \cdot \tanh \kappa\pi < -\alpha/2\right\}$ is mapped by the function $\tilde{f}$ onto $[1, +\infty)$.

If $\kappa \tanh \kappa\pi > -\alpha/2$, then $\tilde{f}(\kappa) < -\cosh \kappa\vartheta$ holds for all $\kappa > 0$ and $\vartheta \in (0, \pi)$.

Proof. The statement for $\alpha \geq 0$ is obvious, assume further that $\alpha < 0$. The first claim follows from the Taylor expansions of the functions involved in $\tilde{f}$, the last uses the equality $\cosh^2 \kappa - \sinh^2 \kappa = 1$. The set determined by the conditions $\cosh \kappa\pi + \frac{\alpha}{4\kappa}\sinh \kappa\pi \geq 1$ and $\kappa \cdot \tanh \kappa\pi < -\alpha/2$ is obviously an interval and $\tilde{f}$ is continuous on it. Since $\cosh \kappa\pi + \frac{\alpha}{4\kappa}\sinh \kappa\pi = 1$ implies $\tilde{f}(\kappa) = 1$ and for $\kappa_0 \cdot \tanh \kappa_0\pi = -\alpha/2$ it holds $\lim_{x \to \kappa_0^-} \tilde{f} = +\infty$, the second claim follows immediately. Finally, if $\kappa \cdot \tanh \kappa\pi > -\alpha/2$, then $\cosh \kappa\pi + \frac{\alpha}{4\kappa}\sinh \kappa\pi > 1$ and $\frac{\alpha}{4\kappa}\sinh \kappa\pi \pm \sqrt{\left(\cosh \kappa\pi + \frac{\alpha}{4\kappa}\sinh \kappa\pi\right)^2 - 1} > 0$, thus $\tilde{f}(\kappa) < -\cosh \kappa\pi < -\cosh \kappa\vartheta$ holds for all $\kappa > 0$ and $\vartheta \in (0, \pi)$. $\qquad \square$

In particular, the first claim concerning $\alpha < 0$ together with the continuity of $\tilde{f}$ implies that if the set $\left\{\kappa : \cosh \kappa\pi + \frac{\alpha}{4\kappa}\sinh \kappa\pi \geq 1\right\}$ is nonempty (and thus an interval), the graph of $\tilde{f}$ on this set lies below the value -1 touching it exactly at the endpoints of this interval.

Corollary 3.4. *If $\alpha \geq 0$, then H^+ has no negative eigenvalues. On the other hand, for $\alpha < 0$ the operator H^+ has at least one negative eigenvalue which lies under the lowest spectral band and above the number $-\kappa_0^2$, where κ_0 is the (unique) solution of $\kappa \cdot \tanh \kappa\pi = -\alpha/2$.*

Proof. The eigenvalues are squares of solutions to the equation $\cosh \kappa\vartheta = \tilde{f}(\kappa)$. The absence of negative eigenvalues for $\alpha \geq 0$ follows directly from the first claim in Proposition 3.3. The same proposition implies that there is exactly one interval mapped by $\tilde{f}$ onto $[1, +\infty)$, hence there is at least one solution of $\cosh \kappa\vartheta = \tilde{f}(\kappa)$ in this interval. $\qquad\square$

3.3 Spectrum of H^- and a summary

The operator H^- which corresponds to the odd part of the wavefunction can be treated in an analogous way. The boundary conditions on the zero circle are now Dirichlet ones,

$$\psi_0 \left(\frac{\pi - \vartheta}{2} \right) = 0, \quad \varphi_0 \left(\frac{\pi + \vartheta}{2} \right) = 0 \,.$$

One can easily find the spectral condition,

$$- \cos k\vartheta = - \cos k\pi + \frac{\sin^2 k\pi}{\frac{\alpha}{4k} \sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k} \sin k\pi \right)^2 - 1}} \,; \qquad (3.13)$$

in comparison with (3.11) corresponding to H^+ there is a difference in the sign of the cosine on the left-hand side. Since we already know the behaviour of the right-hand side, cf. Proposition 3.2, we can infer, similarly as for H^+, that there is at least one solution of (3.13) in each interval I_n except for the case when $- \cos n\vartheta = (-1)^{n-1}$, i.e. when $\vartheta = \frac{n-2\ell}{n}\pi$, $\ell = 1, \ldots, \left[\frac{n}{2} \right]$.

Following the analogy with the symmetric case further we can employ Proposition 3.2 to conclude that in each interval I_n there is at least one solution of $- \cos k\vartheta = f(\kappa)$. The only exception is the interval I_1 for $\alpha < 0$: for $|\alpha|$ sufficiently small it holds $- \cos k\vartheta < f(k)$ in the whole I_1; we will comment on this situation in more detail in the next section devoted to resonances. The negative part of the point spectrum of H^- is determined by the condition

$$- \cosh \kappa\vartheta = - \cosh \kappa\pi - \frac{\sinh^2 \kappa\pi}{\frac{\alpha}{4\kappa} \sinh \kappa\pi \pm \sqrt{\left(\cosh \kappa\pi + \frac{\alpha}{4\kappa} \sinh \kappa\pi \right)^2 - 1}} \,, \quad (3.14)$$

where we set $k = i\kappa$ for $\kappa \in \mathbb{R}^+$. It follows from Proposition 3.3 that (3.14) has a solution for negative α only, and it happens if (i) the positive spectral gap touching zero extends to negative values, and (ii) the bending angle ϑ is small enough. In other words, if there is a number κ_0 solving $\cosh \kappa\pi + \frac{\alpha}{4\kappa} \sinh \kappa\pi = -1$, the energy plot w.r.t. ϑ obtained as the the implicit solutions of (3.14) is a curve departing from $(\vartheta, E) = (0, -\kappa_0^2)$; in the next section we will show that it is analytic and following it one arrives at the point $(\vartheta, E) = (\pi, 1)$.

Let us summarize the discussion of the discrete spectrum. We have demonstrated that for each of the operators $H^\pm$ there generally arises at least one eigenvalue in every spectral gap closure. We have also explained that such an eigenvalue can lapse into a band edge equal to n^2, $n \in \mathbb{N}$, and thus be in fact

absent. The eigenvalues of H^+ and H^- may also coincide, in this case they become a single eigenvalue of multiplicity two. One can check directly that it happens only if

$$k \cdot \tan k\pi = \frac{\alpha}{2}\,.$$

The study of the resonances, performed in the next section, will help us to find more precise results concerning the number of eigenvalues. We will show that there are at *most* two of them in each spectral gap. However, to make the explanation clearer, we refer already at this moment to the Figs. 4–6 illustrating the numerical solution of the spectral condition for different signs of the coupling constant, as well as the resonances of the system.

4 Resonances and analyticity

Proceeding further with the discussion we want to learn more about the angle dependence of the perturbation effects. First we note, however, that the added eigenvalues are not the only consequence of the chain bending. One has to investigate all solutions of (4.1), not only the real ones which correspond to $\sigma_p(H^+)$, but also complex solutions describing *resonances*[2] of $H^\pm$.

Proposition 4.1. *Given a non-integer $k > 0$, the conditions (3.11) and (3.12) for $H^\pm$, respectively, are equivalent to*

$$\frac{\alpha}{2k}(1 \pm \cos k\vartheta \cos k\pi)(\pm \cos k\vartheta + \cos k\pi) = \sin k\pi \cdot (1 \pm 2\cos k\vartheta \cos k\pi + \cos^2 k\vartheta)\,.$$
$$(4.1)$$

Proof. First we note that changing the square root sign in denominator of (3.11) does not give rise to a real solution. Indeed, if the sign of the right-hand side of (3.11) is changed, the obtained expression is of modulus greater than one, hence it cannot be equal to $\cos k\vartheta$. This further implies that one need not specify the sign in the denominator of (3.11) by the sign of $\cos k\pi + \frac{\alpha}{4k}\sin k\pi$, and therefore we can express the square root and subsequently square both sides of the obtained relation. After simple manipulations, we arrive at (4.1); note that for all $k \in \mathbb{R}^+\backslash\mathbb{N}$, the denominator of (3.11) is nonzero. The equivalence of (3.11) and (4.1) for $k \in \mathbb{C}\backslash\mathbb{N}$ is obvious for (4.1) considered with the complex square root, i.e. without restrictions on the sign in the denominator. The argument for H^- is analogous. □

Now we are ready to state and prove the analyticity properties. Since the cases of different symmetries are almost the same, apart of the position of the points where the analyticity fails, we will mention the operator H^+ only.

Proposition 4.2. *Curves given by the implicit equation (4.1) for H^+ are analytic everywhere except at $(\vartheta, k) = (\frac{n+1-2\ell}{n}\pi, n)$, where $n \in \mathbb{N}$, $\ell \in \mathbb{N}_0$,*

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[2]The notion of resonance in the chain-graph system can be introduced in different, mutually equivalent, ways similarly as in [EL07].

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$\ell \leq \left\lceil \frac{n+1}{2} \right\rceil$. *Moreover, the real solution in the n-th spectral gap is given by a function $\vartheta \mapsto k$ which is analytic, except at the points $\frac{n+1-2\ell}{n}\pi$.*

Proof. First we will demonstrate the analyticity of the curves $\vartheta \mapsto k \in \mathbb{C}$. This is easier done using equation (3.11); we have to prove that at each point (ϑ, k) solving the equation $G(\vartheta, k) = 0$ with

$$G(\vartheta, k) = -\cos k\vartheta - \cos k\pi + \frac{\sin^2 k\pi}{\frac{\alpha}{4k} \sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k} \sin k\pi\right)^2 - 1}}$$

the derivative $\frac{\partial G}{\partial \vartheta}$ is nonzero. We have $\frac{\partial G}{\partial \vartheta} = k \cdot \sin(k\vartheta) = 0$ *iff* $\sin k\vartheta = 0$, i.e. $k\vartheta = m\pi$, $m \in \mathbb{Z}$. This implies $G(\vartheta, k) = (-1)^{m+1} - \cos k\pi$, and since $G(\vartheta, k) = 0$ should be satisfied, k is an integer of the same parity as $m + 1$. For $k \in \mathbb{N}$, G is not defined and we use (4.1); it is easy to check that any solution (ϑ, k) of (4.1) with $k \in \mathbb{N}$ corresponds to

$$\vartheta = \frac{k + 1 - 2\ell}{k}\pi, \qquad \ell \in \mathbb{N}, \, \ell \leq \left\lceil \frac{k+1}{2} \right\rceil.$$

To prove that real solutions are analytic functions, it suffices to check that, except at the points $(\varphi, k) = (\frac{n+1-2\ell}{n}\pi, n)$, for each (ϑ, k) solving $F(\vartheta, k) = 0$ with

$$F(\vartheta, k) := \alpha(1 + \cos k\vartheta \cos k\pi)(\cos k\vartheta + \cos k\pi)$$
$$-2k \sin k\pi \cdot (1 + 2\cos k\vartheta \cos k\pi + \cos^2 k\vartheta)$$

it holds $\frac{\partial F}{\partial k} \neq 0$. Computing the derivative one obtains an expression which can be cast into the form

$$2\sin^2 k\pi \cdot (1 + 2\cos k\vartheta \cos k\pi + \cos^2 k\vartheta)^2 +$$
$$+ \alpha \cdot \left[\pi(\cos k\vartheta + \cos k\pi)^4 + \sin^2 k\pi \cdot (\cos k\vartheta + \cos k\pi)^2 + \right.$$
$$\left. + \vartheta \sin^2 k\pi \sin^2 k\vartheta(1 + \cos k(\pi - \vartheta)) + (\pi - \vartheta)\sin^2 k\pi \sin^2 k\vartheta(1 + \cos k\vartheta \cos k\pi) \right].$$

This is always non-negative, and vanishes *iff*

$$(\cos k\pi = 1 \wedge \cos k\vartheta = -1) \vee (\cos k\pi = -1 \wedge \cos k\vartheta = 1),$$

i.e. *iff* $k \in \mathbb{Z}$ and $k\pi = k\vartheta + (2\ell - 1)\pi$, $\ell \in \mathbb{Z}$, proving this the sought claim. $\square$

The resonance dependence on the bending angle ϑ is again visualized on Figs. 4–6 where the real parts are shown; the imaginary parts corresponding to the situation of Fig. 4 are plotted on Fig. 7 below.

5   More on the angle dependence

The above results raise naturally the question about the behaviour of the curves at the singular points $[\vartheta, k] = [\frac{n+1-2\ell}{n}\pi, n]$ with $n \in \mathbb{N}$, $\ell \in \mathbb{N}$, $\ell \leq \left\lceil \frac{n+1}{2} \right\rceil$, where

they touch the band edges and where the eigenvalues and resonances may cross. Now we are going to examine the asymptotic expansion at these points and to look how many curves "stem" from them.

Consider again first the part H^+. Let $k_0 \in \mathbb{N}$ and $\vartheta_0 := \frac{n+1-2\ell}{n}\pi$ for some $\ell \in \mathbb{N}$, and put

$$k := k_0 + \varepsilon, \qquad \vartheta := \vartheta_0 + \delta\,.$$

After substituting into (4.1) with the plus signs and employing Taylor expansions of the cos and sin functions we arrive at the relation

$$\frac{\alpha}{4}\left(k_0^4\delta^4 + 4k_0^3\vartheta_0\delta^3\varepsilon + 6k_0^2\vartheta_0^2\delta^2\varepsilon^2\right) - k_0\pi^3\varepsilon^3 = \mathcal{O}(\delta\varepsilon^3) + \mathcal{O}(\varepsilon^4) + \mathcal{O}(\delta^3\varepsilon)\,.$$

Using the theory of algebroidal functions and Newton polygon, we find that in the neighbourhood of (ϑ_0, k_0), the asymptotical behaviour of solutions is given by the terms of the order δ^4 and ε^3. In other words, up to higher-order term we have $\frac{\alpha}{4}k_0^4\delta^4 = k_0\pi^3\varepsilon^3$, and therefore

$$\left(\frac{\varepsilon\pi}{k_0}\right)^3 = \frac{\alpha}{4}\delta^4\,.$$

Note that $\alpha \in \mathbb{R}$, $k_0 > 0$, $\delta \in \mathbb{R}$, i.e. only ε may be complex here, hence the last equation admits exactly three types of solutions:

- $\varepsilon = \sqrt[3]{\frac{\alpha}{4}\frac{k_0}{\pi}}\,\delta^{4/3}$ (a real solution corresponding to the spectrum)

- $\varepsilon = \mathrm{e}^{\pm \mathrm{i}\frac{2}{3}\pi}\sqrt[3]{\frac{\alpha}{4}\frac{k_0}{\pi}}\,\delta^{4/3}$ (imaginary solutions corresponding to resonances)

Let us remark that since (4.1) has a symmetry with respect to the complex conjugation of k, the imaginary solution come in pairs. This is why we find pairs of curves outside from the real plane, conventionally just one of them is associated with a resonance.

Returning to properties of eigenvalues in a fixed spectral gap, we have so far demonstrated that each real curve describing a solution of (4.1) is a graph of a function analytic except at the singular points, cf. Proposition 4.2. Furthermore, at each singular point only one pair of branches meets (with respect to the variable ϑ); it follows that there is exactly one solution in each spectral gap *closure*. Assuming for definiteness $\alpha > 0$ we can say that the complete graph of solutions of (4.1) has the following structure:

- It consists of curves that are analytic and not intersecting, except at the points $(\vartheta, k) = (\frac{n+1-2\ell}{n}\pi, n)$, where $n \in \mathbb{N}$, $\ell \in \mathbb{N}$, $\ell \leq \left[\frac{n+1}{2}\right]$; these are the only ramification points.

- The real curves branches join the points $(\frac{n+1-2\ell}{n}\pi, n)$ and $(\frac{n+1-2\ell-2}{n}\pi, n)$, i.e. the consecutive points on the lines $k = n \in \mathbb{N}$.

- The curves branches outside the plane $\Im(k) = 0$ join the points $(\frac{\ell}{n-\ell}\pi, n-\ell)$ and $(\frac{\ell+1}{n-\ell-1}\pi, n-\ell-1)$, i.e. the consecutive points laying on the hyperbolas $(\vartheta + \pi)\cdot k = n\cdot\pi$, $k \in \mathbb{R}$, $n \in \mathbb{N}$, n odd, cf. Fig. 7.

Furthermore, we have seen that the behaviour of eigenvalues in vicinity of the singular points is the following,

$$k \approx k_0 + \sqrt[3]{\frac{\alpha}{4} \frac{k_0}{\pi}} \, |\vartheta - \vartheta_0|^{4/3} \,,$$

and this is valid for in the particular case $\vartheta_0 = 0$, $k_0 \in \mathbb{N}$, as well provided the band edge k_0 is odd.

However, H^+ has an eigenvalue near $\vartheta_0 = 0$ also in the gaps adjacent to even numbers. In these cases the curve starts at the point $(0, k_0)$ for k_0 being the solution of $|\cos k\pi + \frac{\alpha}{4k} \sin k\pi| = 1$ in $(n, n+1)$, n even. The asymptotic behaviour of k for ϑ close to zero is then different, namely:

Theorem 5.1. *Suppose that $n \in \mathbb{N}$ is even and k_0 is as described above, i.e. k_0^2 is the right endpoint of the spectral gap adjacent to n^2. Then the behaviour of the solution of* (4.1) *in the neighbourhood of* $(0, k_0)$ *is given by*

$$k = k_0 - C_{k_0, \alpha} \cdot \vartheta^4 + \mathcal{O}(\vartheta^5) \,,$$

where $C_{k_0, \alpha} := \frac{k_0^2}{8\pi} \cdot \left(\frac{\alpha}{4}\right)^3 (k_0 \pi + \sin k_0 \pi)^{-1}$.

Proof. The argument is straightforward, it suffices to use Taylor expansions in (4.1). $\square$

The analogous asymptotic behaviour applies to k^2, the energy distance of the eigenvalue from the band edge is again proportional to ϑ^4 in the leading order. Notice that this is true in any spectral gap, but of course, the error term depends in general on the gap index.

We refrain from discussing in detail the odd part H^- of the Hamiltonian. The corresponding results are practically the same, the only difference is that the roles of the even and odd gaps are interchanged.

Most of what we have discussed above modifies easily to the case of attractive coupling with the obvious changes: for $\alpha < 0$ the spectral gaps lay now *below* the numbers n^2, $n \in \mathbb{N}$. Of particular interest is the spectral gap adjacent to the value one, because with the increase of $|\alpha|$ its lower edge moves towards zero and may become negative for $|\alpha|$ large enough. The even part H^+ has similar properties as before: the eigenvalue curve goes from $(0, 1)$ to (π, k_0), where $k_0 \in (0, 1)$, and there two complex conjugated branches with $\Re(k) > 0$ one of which describes a resonance.

However, the odd part H^- requires a more detailed examination. We know that there is an eigenvalue curve going to the point $[\pi, 1]$. If the entire spectral gap is above zero, this curve joins it with $[0, k_0^2]$, where k_0^2 is the lower edge of the gap. On the other hand, if $|\alpha|$ is large enough the eigenvalue curve starts from $[0, -\kappa_0]$, where $-\kappa_0^2$ is again the lower gap edge; to show that even in this case the curve joins the points $[0, -\kappa_0]$ and $[\pi, 1]$ analytically, it suffices to prove that the solutions of (4.1) with the negative sign preserves analyticity when it crosses the line $k^2 = 0$.

The spectral condition (3.13) for H^- is valid for $k \neq 0$. If we put all terms to the left-hand side denoting it as $\mathcal{G}^-(\vartheta, k)$, i.e.

$$\mathcal{G}^-(\vartheta, k) = -\cos k\vartheta + \cos k\pi - \frac{\sin^2 k\pi}{\frac{\alpha}{4k} \sin k\pi \pm \sqrt{\left(\cos k\pi + \frac{\alpha}{4k} \sin k\pi\right)^2 - 1}}$$

with the sign in the denominator properly chosen, we have $\lim_{k\to 0} \mathcal{G}^-(\vartheta, k) \, k^{-l} = 0$ for $l = 0, 1$ while for $l = 2$ the limit is real-valued and non-vanishing. It follows that to find the behaviour at the crossing point one has to examine the function given implicitly by $\tilde{G}(\vartheta, k) = 0$, where

$$\tilde{G}(\vartheta, k) = \begin{cases} \frac{\mathcal{G}^-(\vartheta, k)}{k^2} & \text{for } k \neq 0 \\ \lim_{k\to 0} \frac{\mathcal{G}^-(\vartheta, k)}{k^2} & \text{for } k = 0 \end{cases}$$

This is continuous and it can be easily checked that it has continuous partial derivatives with respect to ϑ and k in the neighbourhood of any solution of $\tilde{G}(\vartheta, k) = 0$ with $k = 0$. In particular, the derivative w.r.t. ϑ equals $k^{-1} \sin k\vartheta$ for all $k \neq 0$, thus at a point $[\vartheta_0, 0]$ solving $\tilde{G}(\vartheta, k) = 0$ we have

$$\frac{\partial \tilde{G}(\vartheta_0, 0)}{\partial \vartheta} = \lim_{k\to 0} \frac{\sin k\vartheta_0}{k} = \vartheta_0 \neq 0 \,,$$

in other words, the solution of $\tilde{G}(\vartheta, k) = 0$ is analytic also at the point $[\vartheta_0, 0]$. Needless to say, this claim which he have checked directly here can be obtained also by means of the analytic perturbation theory [Ka66].

Finally, note that by Proposition 4.2 the solutions of (4.1) with both the positive and negative signs are analytic in the whole open halfplane $\Re(k) < 0$, and consequently, no resonances curves can be found there.

6 Concluding remarks

We have reasons to believe that the spectral and resonance properties due geometric perturbations of the considered type hold much more generally. In this paper we have decided, however, to treat the present simple example because it allowed us to find a rather explicit solution of the problem.

The problem can be viewed from different perspectives. As an alternative one may interpret the chain graph as a *decoration* of a simple array-type graph, or if you wish, the Kronig-Penney model, in the sense of [Ku05]. The results of the paper then say that *a local modification* of the decoration can produce a discrete spectrum in the gaps and the other effects discussed here.

It is also interesting to draw a parallel between the quantum graphs discussed here and *quantum waveguides*, i.e. Laplacians in tubular domains. Although the nature of the the two system is very different, they nevertheless share some properties, in particular, the existence of bound states below the essential spectrum threshold due to a local bend. This effect is well studied for Dirichlet

quantum waveguides where it is known for a gentle bend the binding energy is proportional to the fourth power of the bending angle [DE95], i.e. it has exactly the same behaviour as described by Theorem 5.1.

Bent quantum waveguides with mixed (or Robin) boundary conditions were also studied [Ji06] and it was shown that the effect of *binding through bending* is present for any repulsive boundary. In our case an eigenvalue below the lowest band exists whenever $\alpha \neq 0$ which inspires another look at the waveguide case. It appears that the argument of [Ji06] works again and proves the existence of curvature-induced bound states in all cases except the Neumann boundary which is an analogue of the case $\alpha = 0$ here.

Acknowledgment

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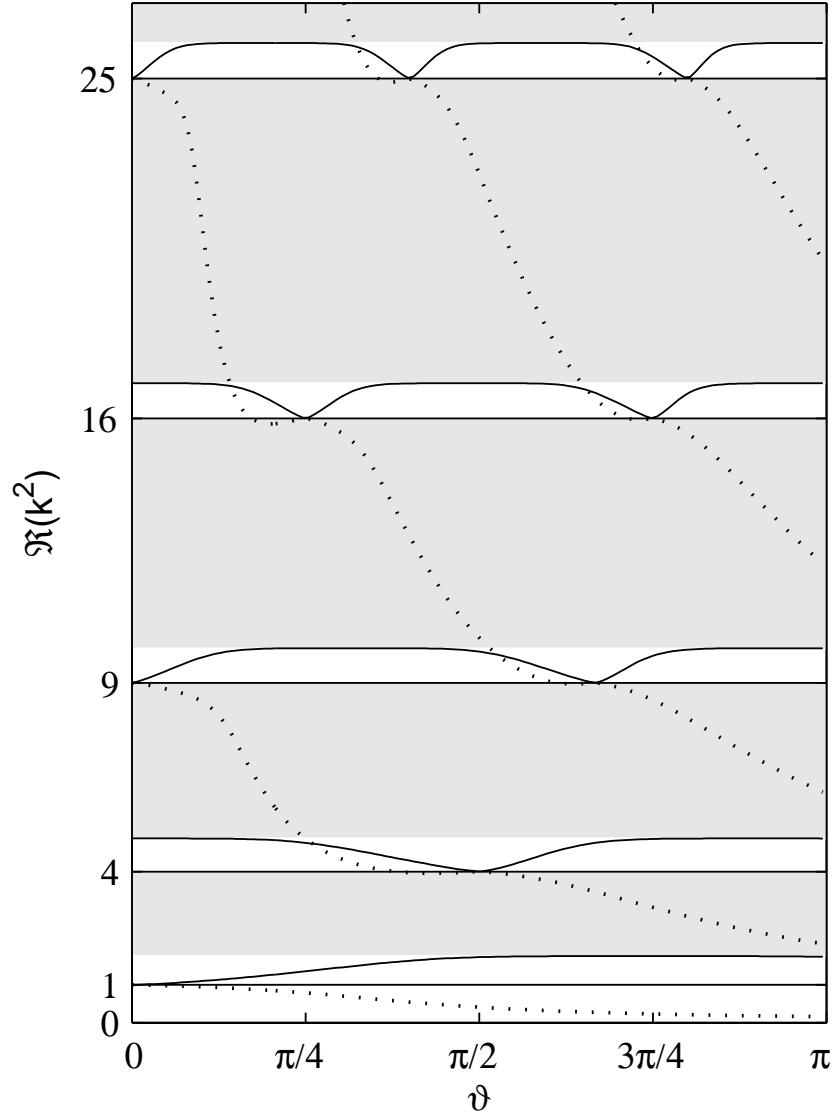[We] J. Weidmann: *Linear Operators in Hilbert Space*, Springer, New York 1980.

Figure 4: The spectrum of H^+ as a function of ϑ for repulsive coupling, $\alpha = 3$. The shaded regions are spectral bands, the dashed lines show real parts of the resonance pole positions discussed in Sec. 4.
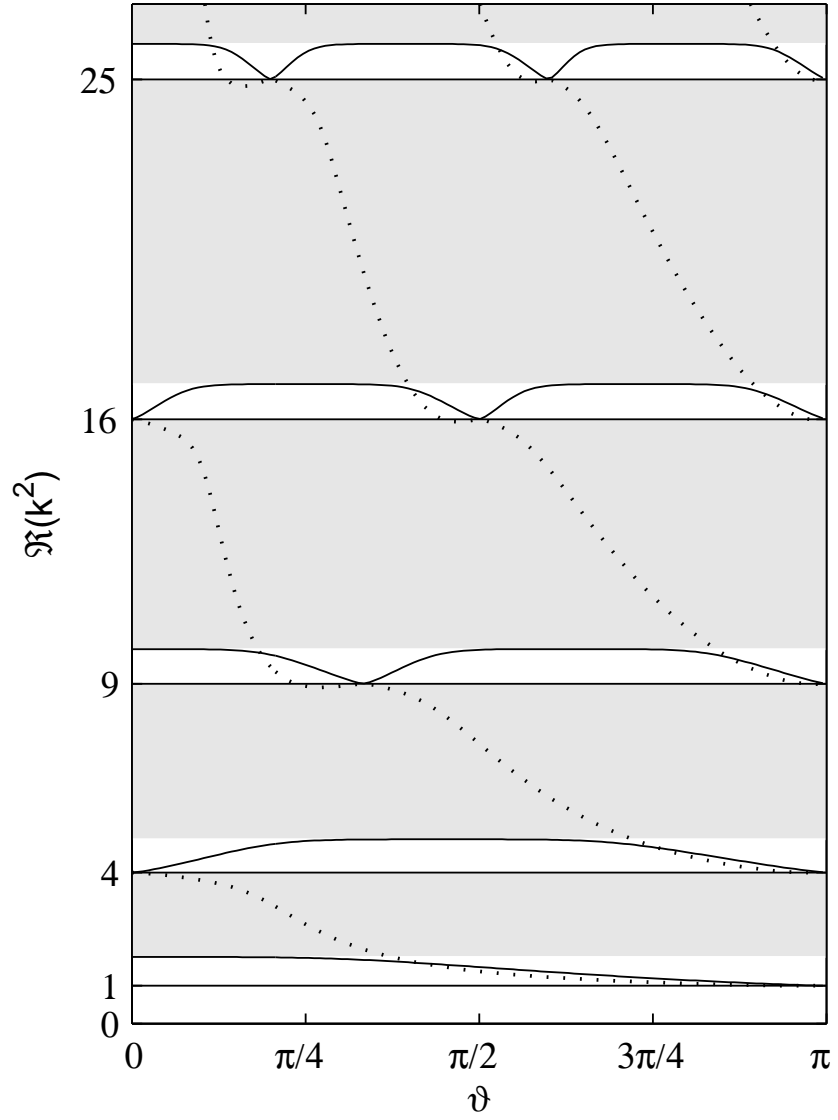
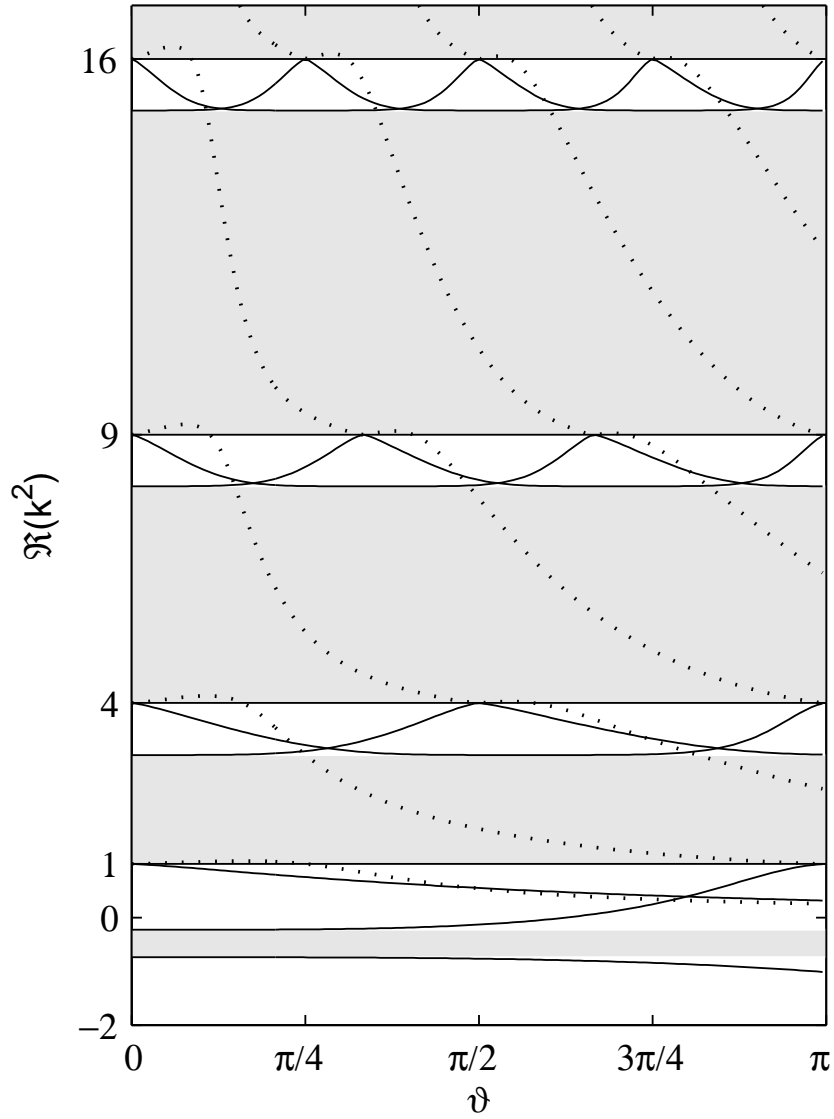Figure 5: The spectrum of H^- in the same setting as in Fig. 4

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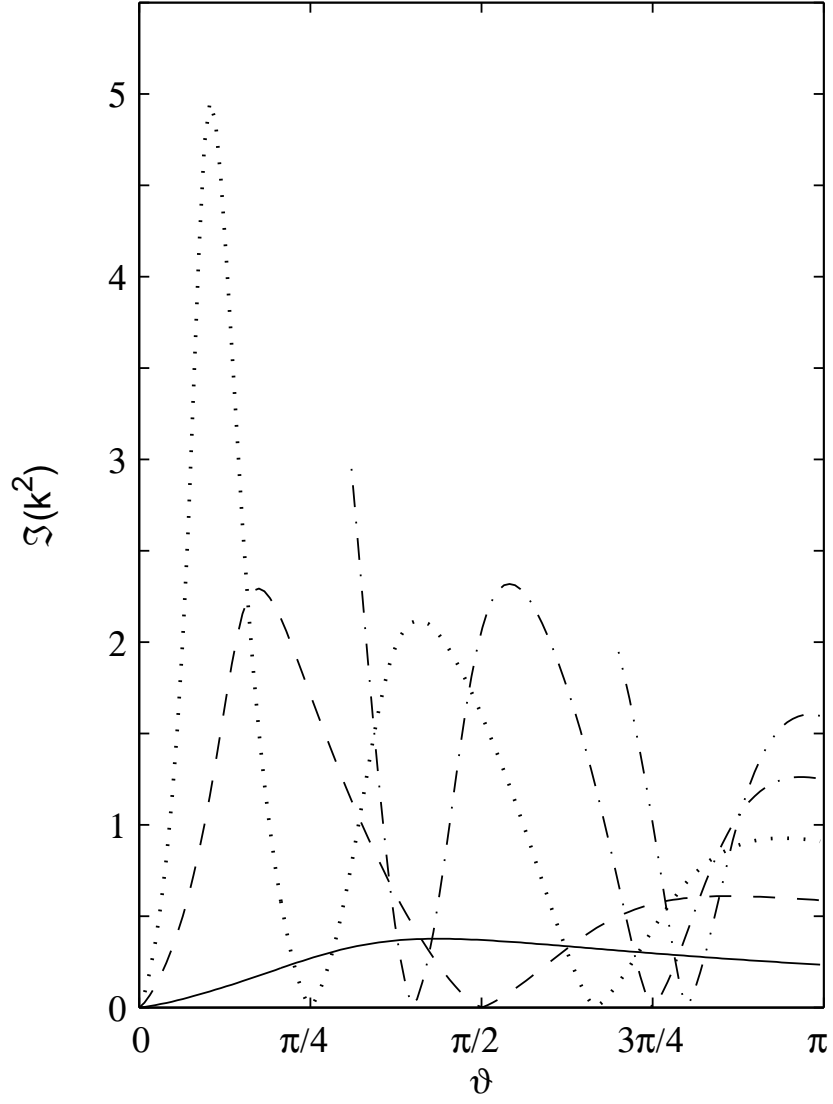Figure 6: The spectrum of H as a function of ϑ for attractive coupling, $\alpha = -3$.

Figure 7: The imaginary parts of resonance pole positions in the same setting as in the previous picture; for the sake of lucidity only the curves corresponding to H^+ are plotted.