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# Non-Hermitian spectral effects in a $\mathcal{PT}$ -symmetric waveguide

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## Abstract

We present a numerical study of the spectrum of the Laplacian in an unbounded strip with  $\mathcal{PT}$ -symmetric boundary conditions. We focus on non-Hermitian features of the model reflected in an unusual dependence of the eigenvalues below the continuous spectrum on various boundary-coupling parameters.

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## 1. Introduction

In the last few years the theory of quasi-Hermitian, pseudo-Hermitian and  $\mathcal{PT}$ -symmetric operators has developed rapidly, and has been shown to provide a huge class of non-Hermitian Hamiltonians with real spectra (cf the pioneering works [4, 23, 24] and review [3] with many references). Because of these recent observations, the condition of self-adjointness of operators representing observables in quantum mechanics may seem to be rather an annoying technicality. However, unless it is met one cannot apply the very powerful machinery of spectral theory based on the spectral theorem.

In particular, one has to restrict to exactly solvable models [19, 21, 22, 25, 27] or to rely on the perturbation and numerical methods to analyse the spectrum of the  $\mathcal{PT}$ -symmetric Hamiltonians. Except for some simple one-dimensional examples [2], the majority of the  $\mathcal{PT}$ -symmetric models studied in the literature have purely discrete spectrum. Perturbation methods are then notably effective in determining the dependence of the eigenvalues on various parameters of the given model. Although the perturbation approach can even prove that the total spectrum is real in some cases [7–9, 20], it is limited in its nature and one usually has to employ numerical techniques in order to obtain a more complete picture of the spectral properties.

In a way motivated by the lack of a well-developed spectral theory for non-self-adjoint operators with non-compact resolvent, in a recent paper [6] Borisov and one of the present authors introduced a new two-dimensional  $\mathcal{PT}$ -symmetric Hamiltonian with a real continuous spectrum. One of the main questions arising within this model is whether the Hamiltonian possesses point spectrum, too. Using some singular perturbation techniques adopted from the theory of quantum waveguides [5, 13], the question was given both positive and negative answers in [6], depending on the nature of the effective  $\mathcal{PT}$ -symmetric interaction in a *weakly-coupled* regime. Moreover, in the case when the point spectrum exists, the weakly-coupled eigenvalues emerging from the continuous spectrum were shown to be real. We refer to section 2 for a precise statement of the spectral results established in [6].

In the present paper, we further analyse the question of the existence of the point spectrum for the Hamiltonian introduced in [6] by *numerical* methods. This enables us to explore quantitative properties of the eigenvalues without the restriction to the weakly-coupled regime. The main emphasis is put on peculiar characteristics of the model which are related to the non-self-adjointness of the underlying Hamiltonian, namely,

- (1) highly *non-monotone* dependence of the eigenvalues on a coupling parameter; as the parameter increases, the eigenvalues emerge from the continuous spectrum, reach a minimum, sometimes disappear in the continuous spectrum, emerge later on again, etc;
- (2) *broken  $\mathcal{PT}$  symmetry*; as the coupling parameter increases, the eigenvalues may emerge from the continuous spectrum as complex-conjugate pairs, collide and become real, move on the real axis, collide again and become complex, etc.

This paper is organized as follows. We begin by recalling the Hamiltonian from [6] and summarize the main spectral properties established there. In particular, we point out some questions the study of [6] has left open. In section 3 we describe the numerical methods we use. The numerical data are then presented and discussed in section 4. In the final section 5 we make some conjectures based on the present study.

## 2. The model, known results and open questions

Given a positive number  $d$ , we introduce an infinite strip  $\Omega := \mathbb{R} \times (0, d)$ , see figure 1. We split the variables consistently by writing  $x = (x_1, x_2)$  with  $x_1 \in \mathbb{R}$  and  $x_2 \in (0, d)$ . Let  $\alpha : \mathbb{R} \rightarrow \mathbb{R}$  be a bounded function; occasionally, we shall denote by the same symbol the function  $x \mapsto \alpha(x_1)$  on  $\Omega$ . The Hamiltonian  $H_\alpha$  we consider in this paper acts simply as the Laplacian in the Hilbert space  $L^2(\Omega)$ , i.e.

$$H_\alpha \Psi := -\Delta \Psi \quad \text{in } \Omega, \tag{1}$$

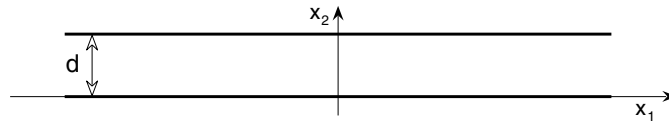
and a non-trivial interaction is introduced by choosing as its domain the set of functions  $\Psi$  from  $W^{2,2}(\Omega)$  satisfying the following Robin-type boundary conditions:

$$\partial_2 \Psi + i\alpha \Psi = 0 \quad \text{on } \partial\Omega. \tag{2}$$

Here,  $W^{2,2}(\Omega)$  denotes the Sobolev space consisting of functions on  $\Omega$  which, together with all their first and second distributional derivatives, are square integrable. As usual, the action of  $H_\alpha$  should be understood in the distributional sense and (2) should be understood in the sense of traces [1].

Under the additional hypothesis that  $\alpha$  possesses a bounded distributional derivative, i.e.  $\alpha \in W^{1,\infty}(\mathbb{R})$ , it was shown in [6] that  $H_\alpha$  is an  $m$ -sectorial operator satisfying

$$H_\alpha^* = H_{-\alpha}, \tag{3}$$



**Figure 1.** A schematic view of an infinite planar waveguide of width  $d$ . The Robin conditions (2) are imposed at the boundary.

where  $H_\alpha^*$  denotes the adjoint of  $H_\alpha$ . (If  $\alpha$  is merely bounded, it is still possible to give a meaning to  $H_\alpha$  by using the quadratic-form approach.) Of course,  $H_\alpha$  is not self-adjoint unless  $\alpha$  vanishes identically. However, relation (3) reflects the  $\mathcal{PT}$  symmetry—or, more generally and more precisely, the  $\mathcal{T}$ -self-adjointness—of  $H_\alpha$ , with  $\mathcal{P}$  and  $\mathcal{T}$  being defined by  $(\mathcal{P}\Psi)(x) := \Psi(d - x)$  and  $\mathcal{T}\Psi := \bar{\Psi}$ , respectively.

An important property of the operator  $H_\alpha$  being  $m$ -sectorial is that it is closed. Then, in particular, the spectrum  $\sigma(H_\alpha)$  is well defined as the set of complex points  $z$  such that  $H_\alpha - z$  is not bijective. The point spectrum  $\sigma_p(H_\alpha)$  equals the set of points  $z$  such that  $H_\alpha - z$  is not injective. The continuous spectrum  $\sigma_c(H_\alpha)$  equals the set of points  $z$  such that  $H_\alpha - z$  is not surjective but the range of  $H_\alpha - z$  is dense in  $L^2(\Omega)$ . Finally, the residual spectrum  $\sigma_r(H_\alpha)$  equals the set of points  $z$  such that  $H_\alpha - z$  is injective but the range of  $H_\alpha - z$  is not dense in  $L^2(\Omega)$ .

In the following theorem, we collect general results about the spectrum of  $H_\alpha$  established in [6].

**Theorem 1.** *Let  $\alpha \in W^{1,\infty}(\mathbb{R})$  and  $\alpha_0 \in \mathbb{R}$ . Then*

- (i)  $\sigma(H_\alpha) \subseteq \{z \in \mathbb{C} : |\arg(z)| \leq \theta\}$  with some  $\theta \in [0, \pi/2)$ ;
- (ii)  $\sigma_r(H_\alpha) = \emptyset$ ;
- (iii)  $\sigma(H_{\alpha_0}) = \sigma_c(H_{\alpha_0}) = [\mu_0^2, \infty)$  where  $\mu_0 := \min\{|\alpha_0|, \pi/d\}$ ;
- (iv) if  $\alpha - \alpha_0 \in C_0(\mathbb{R})$ , then  $\sigma_c(H_\alpha) = [\mu_0^2, \infty)$ ;
- (v) if  $\alpha \in C_0(\mathbb{R})$  is an odd function, then  $\sigma_p(H_\alpha) \subset \mathbb{R}$ .

Here,  $C_0(\mathbb{R})$  denotes the space of continuous functions on  $\mathbb{R}$  with compact support. Note that  $\alpha \in C_0(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$  implies that  $\alpha$  is Lipschitz continuous; conversely, the space of Lipschitz continuous functions on  $\mathbb{R}$  is embedded in  $W^{1,\infty}(\mathbb{R})$ .

The first two properties of theorem 1 are quite general: (i) holds since  $H_\alpha$  is sectorial and (ii) is a consequence of the  $\mathcal{T}$ -self-adjointness (we refer to [6] for more details). Since the spectral problem for the constant case of (iii) can be solved by some sort of ‘separation of variables’ (cf [6], section 4), we shall refer to it as the unperturbed case; it follows from theorem 1 that the corresponding spectrum is purely continuous and positive. As a consequence of (ii), (iv) and (v), we get a result about the reality of the total spectrum in the perturbed case.

**Corollary 1.** *Let  $\alpha \in C_0(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$  be an odd function. Then*

$$\sigma(H_\alpha) \subset \mathbb{R}.$$

The result stated in part (iv) of theorem 1 makes rigorous the heuristic statement that ‘the continuous spectrum depends on the properties of a Hamiltonian interaction at infinity only’. On the other hand, it is well known—and this already for the one-dimensional self-adjoint models [17]—that the point spectrum may be highly unstable under a perturbation

of an operator with non-compact resolvent. In [6], the point spectrum of  $H_\alpha$  was analysed perturbatively in the weakly-coupled regime:

$$\alpha = \alpha_0 + \varepsilon\beta, \quad \text{with } \alpha_0 \in \mathbb{R}, \quad \varepsilon > 0, \quad \beta \in C_0^2(\mathbb{R}), \quad (4)$$

where  $\beta$  is assumed to be real-valued and  $\varepsilon$  plays the role of the small parameter. Here,  $C_0^2(\mathbb{R})$  denotes the space of functions on  $\mathbb{R}$  which, together with all their first and second derivatives, are continuous and have compact support. The main interest was focused on the existence and asymptotic behaviour of the eigenvalues emerging from the threshold  $\mu_0^2$  of the continuous spectrum due to the perturbation of  $H_{\alpha_0}$  by  $\varepsilon\beta$ .

Before stating the main results of [6] about the weakly-coupled eigenvalues, we need to introduce some notation. Recalling the definition of  $\mu_0$  from theorem 1(iii), we next define

$$\mu_1 := \max\{|\alpha_0|, \pi/d\} \quad \text{and} \quad \mu_j := \pi j/d \quad \text{for } j \geq 2.$$

To these numbers we associate a family of functions  $\{\psi_j\}_{j=0}^\infty$  by

$$\psi_j(x_2) := \cos(\mu_j x_2) - i \frac{\alpha_0}{\mu_j} \sin(\mu_j x_2). \quad (5)$$

Let  $\{v_j\}_{j=0}^\infty$  be a sequence of auxiliary functions given by

$$v_j(x_1) := \begin{cases} -\frac{1}{2} \int_{\mathbb{R}} |x_1 - t_1| \beta(t_1) dt_1 & \text{if } j = 0, \\ \frac{1}{2\sqrt{\mu_j^2 - \mu_0^2}} \int_{\mathbb{R}} e^{-\sqrt{\mu_j^2 - \mu_0^2}|x_1 - t_1|} \beta(t_1) dt_1 & \text{if } j \geq 1. \end{cases}$$

Finally, denoting  $\langle f \rangle = \int_{\mathbb{R}} f(x_1) dx_1$  for any  $f \in L^1(\mathbb{R})$ , we introduce a constant  $\tau$ , depending on  $\beta$ ,  $d$  and  $\alpha_0$ , by

$$\tau := \begin{cases} 2\alpha_0^2 \langle \beta v_0 \rangle + \frac{2\alpha_0}{d} \sum_{j=1}^\infty \frac{\mu_j^2 \langle \beta v_j \rangle}{\mu_j^2 - \mu_0^2} \tan \frac{\alpha_0 d + j\pi}{2} & \text{if } |\alpha_0| < \frac{\pi}{d}, \\ \frac{2\alpha_0 \pi^2 \cot \frac{\alpha_0 d}{2}}{(\mu_1^2 - \mu_0^2) d^3} \langle \beta v_1 \rangle + \frac{8\pi^2}{(\mu_1^2 - \mu_0^2) d^4} \sum_{j=1}^\infty \frac{\mu_{2j}^2 \langle \beta v_{2j} \rangle}{\mu_{2j}^2 - \mu_1^2} & \text{if } |\alpha_0| > \frac{\pi}{d}. \end{cases} \quad (6)$$

Now we are in a position to take over from [6] the following theorem.

**Theorem 2.** *Let  $\alpha$  be given by (4).*

(A) *If  $\alpha_0 = 0$ , then  $H_\alpha$  has no eigenvalues converging to  $\mu_0^2$  as  $\varepsilon \rightarrow 0$ .*

(B) *Let  $0 < |\alpha_0| < \pi/d$ .*

(1) *If  $\alpha_0 \langle \beta \rangle < 0$ , then there exists the unique eigenvalue  $\lambda_\varepsilon$  of  $H_\alpha$  converging to  $\mu_0^2$  as  $\varepsilon \rightarrow 0$ . This eigenvalue is simple and real, and satisfies the asymptotic formula*

$$\lambda_\varepsilon = \mu_0^2 - \varepsilon^2 \alpha_0^2 \langle \beta \rangle^2 + 2\varepsilon^3 \alpha_0 \tau \langle \beta \rangle + \mathcal{O}(\varepsilon^4). \quad (7)$$

(2) *If  $\alpha_0 \langle \beta \rangle > 0$ , then  $H_\alpha$  has no eigenvalues converging to  $\mu_0^2$  as  $\varepsilon \rightarrow 0$ .*

(3) *If  $\langle \beta \rangle = 0$  and  $\tau > 0$ , then there exists the unique eigenvalue  $\lambda_\varepsilon$  of  $H_\alpha$  converging to  $\mu_0^2$  as  $\varepsilon \rightarrow 0$ . This eigenvalue is simple and real, and satisfies the asymptotics*

$$\lambda_\varepsilon = \mu_0^2 - \varepsilon^4 \tau^2 + \mathcal{O}(\varepsilon^5). \quad (8)$$

(4) *If  $\langle \beta \rangle = 0$  and  $\tau < 0$ , then  $H_\alpha$  has no eigenvalues converging to  $\mu_0^2$  as  $\varepsilon \rightarrow 0$ .*

(C) *Let  $|\alpha_0| > \pi/d$  and  $\alpha_0 d/\pi \notin \mathbb{Z}$ .*

(1) *If  $\tau > 0$ , then there exists the unique eigenvalue  $\lambda_\varepsilon$  of  $H_\alpha$  converging to  $\mu_0^2$  as  $\varepsilon \rightarrow 0$ , it is simple and real, and satisfies the asymptotics (8).*

(2) *If  $\tau < 0$ , then  $H_\alpha$  has no eigenvalues converging to  $\mu_0^2$  as  $\varepsilon \rightarrow 0$ .*

The method of [6] gives also the asymptotic expansion of the eigenfunctions corresponding to the weakly-coupled eigenvalues.

**Theorem 3.** *The eigenfunction  $\Psi_\varepsilon$  corresponding to any eigenvalue  $\lambda_\varepsilon$  from theorem 2 can be chosen so that it satisfies the asymptotics*

$$\Psi_\varepsilon(x) = \psi_0(x_2) + \mathcal{O}(\varepsilon) \tag{9}$$

in  $W^{2,2}(\Omega \cap \{x : |x_1| < a\})$  for each  $a > 0$ , and behaves at infinity as

$$\Psi_\varepsilon(x) = \exp^{-\sqrt{\mu_0^2 - \lambda_\varepsilon} |x_1|} \psi_0(x_2) + \mathcal{O}(\exp^{-\sqrt{\mu_0^2 - \lambda_\varepsilon} |x_1|}), \quad x_1 \rightarrow +\infty. \tag{10}$$

Theorems 1–3 summarizing the spectral analysis performed in [6] leave open the following particular questions:

- (Q1) Can the cases (B4) and (C2) of theorem 2 occur? That is, can the constant  $\tau$  be negative for a certain combination of  $d, \alpha_0$  and  $\beta$ ? (Sufficient conditions for the positivity of  $\tau$  exist ([6], propositions 2.1 and 2.2).)
- (Q2) What happens in the case (C) of theorem 2 if the condition  $\alpha_0 d / \pi \notin \mathbb{Z}$  is not satisfied? Is it just a technical hypothesis?
- (Q3) Is there any point spectrum in the case of corollary 1?
- (Q4) What is the dependence of the weakly-coupled eigenvalues of theorem 2 as the parameter  $\varepsilon$  increases?
- (Q5) Do the eigenvalues remain real for large  $\varepsilon$ ?
- (Q6) Can one have more eigenvalues? Can they be degenerate? What is the dependence of the number of eigenvalues on  $\varepsilon$ ?
- (Q7) Are there any eigenvalues emerging from other thresholds  $\mu_j^2, j \geq 1$ ? Can they emerge from other points of the continuous spectrum, different from the thresholds  $\mu_j^2, j \geq 0$ ?

The main goal of the present paper is to provide answers to some of these questions by a numerical study of the spectral problem.

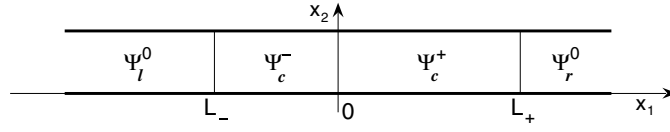
### 3. Numerical methods

In order to get the dependence of the bound states on parameters, such as  $\varepsilon, d, \alpha_0$ , etc, numerically we used two independent methods. When  $\alpha$  is a simple step-like function (e.g. symmetric or asymmetric square well), we treat the problem by the mode matching method. It takes into account the asymptotic behaviour of solution explicitly and can serve thus as a useful check when we apply the other method, namely, the spectral method. This method is more robust and we use it for more general  $\alpha$ . We arrived at an excellent agreement in cases when both methods are applicable.

#### 3.1. Mode matching method

Let us begin with mode matching. The most general situation we want to describe is shown in figure 2. Fix the negative and positive numbers  $L_-$  and  $L_+$ , respectively. In the asymptotic regions, i.e.  $x_1 < L_-$  and  $L_+ < x_1$ , we assume  $\alpha(x_1) = \alpha_0$ , while in the central parts we have  $\alpha(x_1) = \alpha_-$  if  $L_- < x_1 < 0$  and  $\alpha(x_1) = \alpha_+$  if  $0 < x_1 < L_+$ .

Let  $\{\mu_j^\pm\}_{j=0}^\infty$  denote the sequence of numbers  $\{\mu_j\}_{j=0}^\infty$  with  $\alpha_0$  being replaced by  $\alpha_\pm$ . In the same way we define the sequence of functions  $\{\psi_j^\pm\}_{j=0}^\infty$  by replacing  $\alpha_0$  by  $\alpha_\pm$  in (5). In order to make the notation more consistent, hereafter we write  $\mu_j^0$  and  $\psi_j^0$  instead of  $\mu_j$  and  $\psi_j$ , respectively, and introduce a common index  $\iota \in \{0, +, -\}$ .



**Figure 2.** The mode matching approach. A particular *ansatz* (11) for an eigenfunction  $\Psi$  of  $H_\alpha$  corresponding to  $\lambda$  is chosen in each subregion and the smooth matching (12) is required at the boundaries separating the subregions.

In each of the regions where  $\alpha$  is constant, the spectral problem  $-\Delta\Psi = \lambda\Psi$ , with  $\Psi$  satisfying the required boundary conditions, can be solved explicitly ([6], section 4) by expanding  $\Psi$  into the ‘transverse basis’  $\{\psi_j^\iota\}_{j=0}^\infty$ , where  $\iota$  depends on the region. More specifically, we use the following *ansatz* for an eigenfunction  $\Psi$  of  $H_\alpha$  corresponding to  $\lambda$ :

$$\Psi(x) = \begin{cases} \Psi_l^0(x) := \sum_{j=0}^\infty d_j e^{\sqrt{(\mu_j^0)^2 - \lambda}x_1} \psi_j^0(x_2) & \text{if } x_1 \in (-\infty, L_-), \\ \Psi_c^-(x) := \sum_{j=0}^\infty c_j \phi_j^-(x_1) \psi_j^-(x_2) & \text{if } x_1 \in (L_-, 0), \\ \Psi_c^+(x) := \sum_{j=0}^\infty b_j \phi_j^+(x_1) \psi_j^+(x_2) & \text{if } x_1 \in (0, L_+), \\ \Psi_r^0(x) := \sum_{j=0}^\infty a_j e^{-\sqrt{(\mu_j^0)^2 - \lambda}x_1} \psi_j^0(x_2) & \text{if } x_1 \in (L_+, +\infty), \end{cases} \quad (11)$$

where

$$\phi_j^\pm(x_1) := \cos(\sqrt{\lambda - (\mu_j^\pm)^2}x_1) + B_\pm \sin(\sqrt{\lambda - (\mu_j^\pm)^2}x_1).$$

The standard elliptic regularity theory implies that any weak solution  $\Psi$  to  $-\Delta\Psi = \lambda\Psi$  is necessarily infinitely smooth in the interior of  $\Omega$ . In particular, we must match the functions from the *ansatz* smoothly at  $x_1 = L_-, 0, L_+$ , i.e. we require

$$\begin{aligned} \Psi_l^0(L_-, x_2) &= \Psi_c^-(L_-, x_2), & \partial_1 \Psi_l^0(L_-, x_2) &= \partial_1 \Psi_c^-(L_-, x_2), \\ \Psi_c^-(0, x_2) &= \Psi_c^+(0, x_2), & \partial_1 \Psi_c^-(0, x_2) &= \partial_1 \Psi_c^+(0, x_2), \\ \Psi_c^+(L_+, x_2) &= \Psi_r^0(L_+, x_2), & \partial_1 \Psi_c^+(L_+, x_2) &= \partial_1 \Psi_r^0(L_+, x_2), \end{aligned} \quad (12)$$

for every  $x_2 \in (0, d)$ .

If  $\{\psi_j^\iota\}_{j=0}^\infty$  formed an orthonormal family, the next step would consist in employing the orthonormality and reducing (12) into a system of algebraic equations for the coefficients  $a_j, b_j, c_j, d_j$ . However, since the family  $\{\psi_j^\iota\}_{j=0}^\infty$  is actually formed by eigenfunctions of a transverse eigenvalue problem which is not Hermitian (unless  $\alpha_\iota = 0$ ), it is clear that the functions  $\psi_j^\iota$  are not mutually orthogonal in general. Instead, we use the property that  $\{\psi_j^\iota\}_{j=0}^\infty$  and  $\{\phi_j^\iota\}_{j=0}^\infty$  form a complete biorthonormal pair [19], where  $\phi_j^\iota$  are properly normalized eigenfunctions of the adjoint transverse problem:

$$\phi_j^\iota(x_2) := \overline{A_j^\iota \psi_j^\iota(x_2)}.$$

The normalization constants can be chosen as follows:

$$A_{j_0}^\iota := \frac{2i\alpha_\iota}{1 - \exp(-2i\alpha_\iota d)}, \quad A_{j_1}^\iota := \frac{2(\mu_1^\iota)^2}{[(\mu_1^\iota)^2 - \alpha_\iota^2]d}, \quad A_j^\iota := \frac{2(\mu_j^\iota)^2}{[(\mu_j^\iota)^2 - \alpha_\iota^2]d},$$

where  $j \geq 2$ ,  $(j_0, j_1) = (0, 1)$  if  $|\alpha_l| < \pi/d$  and  $(j_0, j_1) = (1, 0)$  if  $|\alpha_l| > \pi/d$  (if  $\alpha_l = 0$ , the fraction in the definition of  $A_{j_0}^l$  should be understood as the expression obtained after taking the limit  $\alpha_l \rightarrow 0$ ). Then, in particular, we have

$$\forall i, j \in \mathbb{N}, \quad (\phi_i^l, \psi_j^l) = \delta_{ij}, \tag{13}$$

where  $(\cdot, \cdot)$  denotes the inner product in  $L^2((0, d))$ , antilinear in the first factor and linear in the second one.

Now, multiplying (12) by  $\overline{\phi_i^0}$ , integrating over  $x_2 \in (0, d)$  and employing (13) in the asymptotic regions, we can eliminate the coefficients  $a_j$  and  $d_j$  by means of the relations

$$\begin{aligned} a_i e^{-\sqrt{(\mu_i^0)^2 - \lambda}L_+} &= \sum_{j=0}^{\infty} b_j \varphi_j^+(L_+) (\phi_i^0, \psi_j^+), \\ d_i e^{\sqrt{(\mu_i^0)^2 - \lambda}L_-} &= \sum_{j=0}^{\infty} c_j \varphi_j^-(L_-) (\phi_i^0, \psi_j^-), \end{aligned} \tag{14}$$

for every  $i \in \mathbb{N}$ , and reduce thus the number of conditions to be fulfilled. We finally arrive at an infinite-dimensional homogeneous system

$$\begin{pmatrix} m_{11} & m_{12} & 0 & 0 \\ m_{21} & 0 & m_{33} & 0 \\ 0 & 0 & m_{33} & m_{34} \\ 0 & m_{42} & 0 & m_{44} \end{pmatrix} \begin{pmatrix} b \\ c \\ bB_+ \\ cB_- \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{15}$$

Here,  $b, c$  denote the infinite vectors formed by  $b_j, c_j$ , respectively, and the submatrices  $m_{\mu\nu}$  are given by

$$\begin{aligned} m_{11} &:= (\phi_i^0, \psi_j^+), & m_{33} &:= \sqrt{\lambda - (\mu_j^+)^2} (\phi_i^0, \psi_j^+), \\ m_{12} &:= -(\phi_i^0, \psi_j^-), & m_{34} &:= -\sqrt{\lambda - (\mu_j^-)^2} (\phi_i^0, \psi_j^-), \\ m_{21} &:= \left( \sqrt{(\mu_i^0)^2 - \lambda} \cos(L_+ \sqrt{\lambda - (\mu_j^+)^2}) \right. \\ &\quad \left. - \sqrt{\lambda - (\mu_j^+)^2} \sin(L_+ \sqrt{\lambda - (\mu_j^+)^2}) \right) (\phi_i^0, \psi_j^+), \\ m_{23} &:= \left( \sqrt{(\mu_i^0)^2 - \lambda} \sin(L_+ \sqrt{\lambda - (\mu_j^+)^2}) \right. \\ &\quad \left. + \sqrt{\lambda - (\mu_j^+)^2} \cos(L_+ \sqrt{\lambda - (\mu_j^+)^2}) \right) (\phi_i^0, \psi_j^+), \\ m_{42} &:= \left( \sqrt{(\mu_i^0)^2 - \lambda} \cos(L_- \sqrt{\lambda - (\mu_j^-)^2}) \right. \\ &\quad \left. + \sqrt{\lambda - (\mu_j^-)^2} \sin(L_- \sqrt{\lambda - (\mu_j^-)^2}) \right) (\phi_i^0, \psi_j^-), \\ m_{44} &:= \left( \sqrt{(\mu_i^0)^2 - \lambda} \sin(L_- \sqrt{\lambda - (\mu_j^-)^2}) \right. \\ &\quad \left. - \sqrt{\lambda - (\mu_j^-)^2} \cos(L_- \sqrt{\lambda - (\mu_j^-)^2}) \right) (\phi_i^0, \psi_j^-), \end{aligned}$$

where the right-hand sides should be understood as the infinite matrices formed by the respective coefficients for  $i, j \in \mathbb{N}$ . Our numerical approximation then consists in



approximating the infinite system by using finite submatrices for  $i, j \in \{0, \dots, N\}$  with  $N$  large enough.

In order to have a non-trivial solution, we require

$$\det \begin{pmatrix} m_{11} & m_{12} & 0 & 0 \\ m_{21} & 0 & m_{23} & 0 \\ 0 & 0 & m_{33} & m_{34} \\ 0 & m_{42} & 0 & m_{44} \end{pmatrix} = 0, \tag{16}$$

which gives an implicit equation for  $\lambda$  as the unknown. Having found  $\lambda$ , we can then calculate the coefficients  $a_j, b_j, c_j, d_j, B_{\pm,j}$  from (15) and (14).

If  $\alpha_+ = \alpha_-$  and  $L_+ = -L_-$ , i.e.  $\alpha$  is a symmetric square well, then (16) can be reduced to

$$\det \begin{pmatrix} m_{21} + m_{42} & 0 \\ 0 & m_{23} - m_{44} \end{pmatrix} = 0.$$

The solutions have different symmetry with respect to  $x_1 \mapsto -x_1$ , the even solutions are formed only of cosines, the odd of sines.

**Remark.** In principle, it is possible to extend the present method to an arbitrary piecewise constant function  $\alpha$ , provided that the number of matching interfaces is finite. On the other hand, the more matching conditions the bigger is the size of the matrix of (15) and thus the higher (numerical) price one must pay.

### 3.2. Spectral method

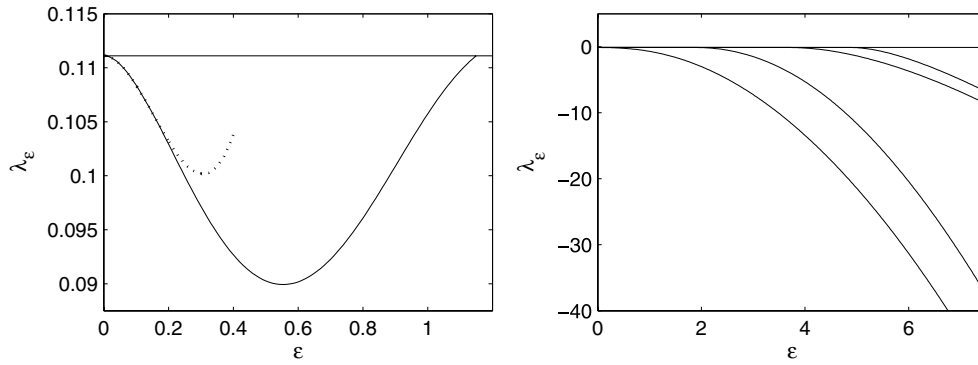
In order to treat the waveguide with a general  $\alpha$  in the boundary conditions, we decided to use spectral collocation methods. They provide a reliable and rapidly converging tool easily applicable to our model. A very useful software suite has already been published [26]. It could be adapted to this problem. We approximate the operator by a series of operators defined on a finite domain  $[x_1^{\min}, x_1^{\max}] \times [0, d]$  with the Dirichlet boundary conditions on  $\{x_1^{\min}\} \times [0, d]$  and  $\{x_1^{\max}\} \times [0, d]$ .

First, we can form the differentiation matrices in each variable separately and then combine them to the two-dimensional problem. The infinite domain in  $x_1$ -variable suggests that we could approximate it by grid points chosen as the roots of Hermite polynomials and as an interpolant we take the Lagrange polynomial. There is an additional parameter (the real line can be mapped to itself by a change of variable  $x_1 = b\tilde{x}_1, b > 0$ ), which can be used to optimize the choice of the grid points together with the variation of the number of roots  $N_1$ . The roots span the interval  $[\xi_1, \xi_{N_1}], -\xi_1 = \xi_{N_1}$ , cluster around the origin, and grow as  $\xi_{N_1} = \mathcal{O}(\sqrt{N_1})$  for  $N_1 \rightarrow \infty$ .

Another possibility is to use the Fourier differencing. We form a uniform grid in  $[-x_1^{\max}, x_1^{\max}]$  and since the solutions decay exponentially, we can theoretically extend it periodically across this interval to the whole  $\mathbb{R}$ . The interpolant is a trigonometric function.

In both approaches the interpolant is an infinitely differentiable function. Deriving it and taking the derivatives in the grid points we get the differentiation matrices. Imposing the homogeneous Dirichlet boundary conditions consists in deleting the first and the last rows and columns of the differentiation matrices.

The transversal variable is confined to a finite interval  $[0, d]$  and it is possible to scale it to  $[-1, 1]$ . To implement the boundary conditions, we prefer to incorporate them into the interpolant. It requires to use the Hermite interpolation, which takes into account derivative values in addition to function values. The use of the roots of Chebyshev polynomials



**Figure 3.** Comparison of the dependence of eigenvalues on  $\varepsilon$  for  $\mathcal{PT}$ -symmetric and self-adjoint waveguides. The left figure shows the  $\mathcal{PT}$ -symmetric case with  $\alpha(x_1) = 1/3 - \varepsilon \exp(-x_1^2)$ . Here the solid (respectively, dotted) curve represents the eigenvalue (respectively, the asymptotic formula (7) up to the  $\varepsilon^3$ -term). The right figure shows the eigencurves in the corresponding self-adjoint situation, obtained by replacing  $i\alpha \mapsto \alpha$  in (2).  $d = 2$  in both cases.

$\eta_k = \cos((k - 1)\pi/(N_2 - 1)), k = 1, \dots, N_2$ , as the grid points is common here. For details we refer the reader to [26].

Now, it remains to form differentiation matrices that correspond to partial derivatives entering the Laplacian. Having set up a grid in each direction, we combine them into the tensor product grid. Then a closer inspection shows that  $\partial_1^2 \rightarrow D^{(2)}(x_1) \otimes \mathbf{I}$ , where  $\mathbf{I}$  is an  $N_2 \times N_2$  identity matrix and  $\partial_2^2$  is constructed in a similar way (it is necessary to take into account that the boundary conditions change with  $x_1$ ).

Applying the spectral discretization, we converted the search for eigenvalues of  $H_\alpha$  to a matrix eigenvalue problem.

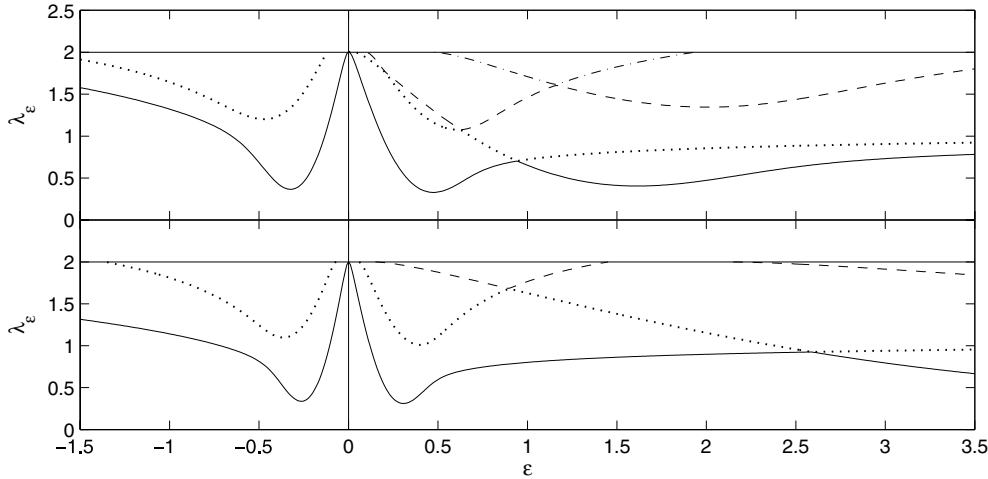
#### 4. Discussion of numerical results

The existence of eigenvalues below the threshold of the continuous spectrum and their behaviour for weak perturbations was already proved in [6]. Our calculations confirm it and demonstrate that the spectrum of eigenvalues is considerably richer.

A typical dependence of an eigenvalue on the perturbation parameter  $\varepsilon$  is shown in figure 3. Here we perturbed a waveguide of width  $d = 2$  and  $\alpha_0 = 1/3$  by a Gaussian shape, i.e. we took  $\beta(x_1) = -\exp(-x_1^2)$  in (4). Since  $0 < \alpha_0 < \pi/d$  and  $\langle \beta \rangle < 0$ , we deal with the case (B1) of theorem 2. We observe that the asymptotic expansion (7) is fairly good. It is striking, however, that the dependence of the eigenvalue on  $\varepsilon$  is highly non-monotonic: the eigenvalue appears at some value of  $\varepsilon$  (in this case it is  $\varepsilon = 0$ ), reaches a minimum and then returns to the continuous spectrum. We found such a behaviour in all the cases we studied, namely, various shapes of symmetric and asymmetric wells, and Gaussians times polynomials. This provides an interesting answer to (Q4) from the end of section 2.

It is worth noting that this behaviour differs from that in the self-adjoint waveguide obtained simply by omitting the imaginary unit in (2). As shows the second graph in figure 3, in the self-adjoint case all the energy levels are increasingly more bound when  $\varepsilon$  increases.

On the other hand, we checked that the eigenvalues are decreasing as functions of  $L := \pm L_\pm$  for the symmetric square-well profile  $\alpha_+ = \alpha_-$  of section 3.1 in the regime  $0 < \alpha_\pm < \alpha_0 < \pi/d$ . This is reasonable to expect since as  $L \rightarrow \infty$  the eigenvalues



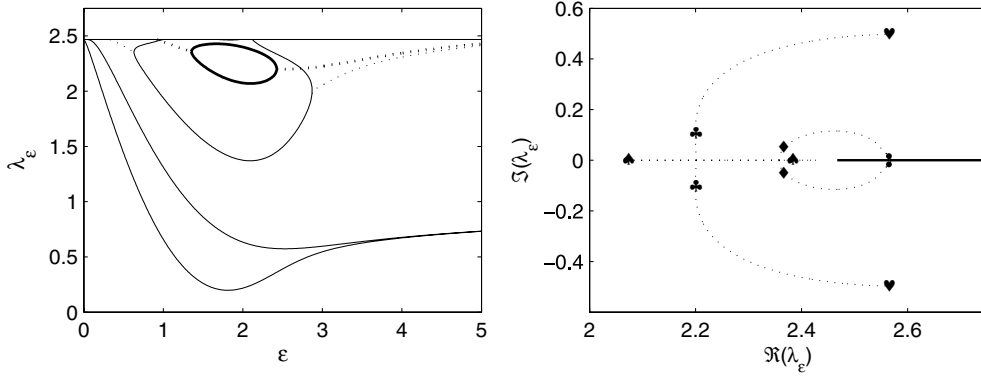
**Figure 4.** Dependence of eigenvalues on  $\varepsilon$  in the critical case  $\langle \beta \rangle = 0, \tau > 0$ . Here,  $\alpha(x_1) = \sqrt{2} - \varepsilon(x_1^2 + bx_1 - 5) \exp(-x_1^2/10)$  and  $d = 2$ . The upper figure corresponds to  $b = 1.5$  and the lower one to  $b = 3.25$ . All the crossings are avoided.

should approach  $(\alpha_{\pm})^2$ , i.e. the threshold of the continuous spectrum of the unperturbed waveguide  $H_{\alpha_{\pm}}$ .

An answer to questions from (Q6) is provided in figure 4. It corresponds to the critical case (B3) of theorem 2 with  $\beta(x_1) = -(x_1^2 + bx_1 - 5) \exp(-x_1^2/10)$ ,  $\alpha_0 = \sqrt{2}$  and  $d = 2$ ; the parameter  $b$  changes the asymmetry of  $\beta$ . In addition to the weakly-coupled eigenvalue of theorem 2, there are also other eigenvalues emerging from the continuous spectrum as  $\varepsilon$  increases. The lower figure (case  $b = 3.25$ ) shows that there might be eigenvalues existing in disjoint intervals of  $\varepsilon$  (the dashed curve). By diminishing  $\alpha_0$ , we can achieve the situation when there is only one eigenvalue with a similar behaviour: it emerges from the threshold of continuous spectrum (at  $\varepsilon = 0$ ), reaches a minimum, returns to the continuum, reappears later on and returns finally to the continuum.

Another typical feature is that the energy levels do not cross. We saw always avoided crossings (at least in the unbroken  $\mathcal{PT}$  regime), i.e. the order of levels remains unchanged and the non-monotonicity of the excited eigenvalues is preserved.

The spectrum in figure 5 is remarkable from two points of view. First, it corresponds to the case of (Q2) from the end of section 2, since the constant  $\alpha_0$  is chosen so that its square coincides with the threshold of the continuous spectrum, which is  $(\pi/2)^2 \approx 2.47$  for  $d = 2$ . Second, we see that this situation provides a negative answer to (Q5), i.e. the  $\mathcal{PT}$  symmetry can be broken, and a partial answer to (Q7). Let us comment on the behaviour marked by the thick curve in the left figure. There is a critical value of the parameter  $\varepsilon$  for which there emerges a pair of complex conjugate eigenvalues from the continuous spectrum (we suspect that they emerge due to a collision of two embedded eigenvalues). As  $\varepsilon$  increases, the eigenvalues propagate in the complex plane (this is indicated by the dotted curves joining the discs and diamonds in the right figure; the dotted curve in the left figure traces the common real parts of the eigenvalues) till they collide on the real axis and become real. Then they move on the real axis (as the spades) in opposite directions till they reach turning points (each of them for different value of  $\varepsilon$ ), starts to approach each other, coalesce again and continue as a pair of complex conjugate eigenvalues (indicated by the clubs and hearts) until they disappear



**Figure 5.** Broken  $\mathcal{PT}$  symmetry. The left figure shows the dependence of eigenvalues on  $\varepsilon$  in the case  $\alpha(x_1) = \pi/2 - \varepsilon \exp(-x_1^2/10)$  and  $d = 2$ . Here the dotted line is used to plot the real part of the eigenvalues if they form complex conjugate pairs instead of being real. The dotted line in the right figure shows the trajectory in the complex plane of the pair of (complex) eigenvalues corresponding to the thick curve in the left figure. The thick line in the right figure marks the continuous spectrum. The pairs of symbols show positions of eigenvalues for different values of  $\varepsilon$ : 0.1 (disc), 1.3 (diamond), 2.1 (spade), 2.5 (club) and 8 (heart). An animation can be found at the website [18] or from [stacks.iop.org/JPhysA/41/244013](http://stacks.iop.org/JPhysA/41/244013).

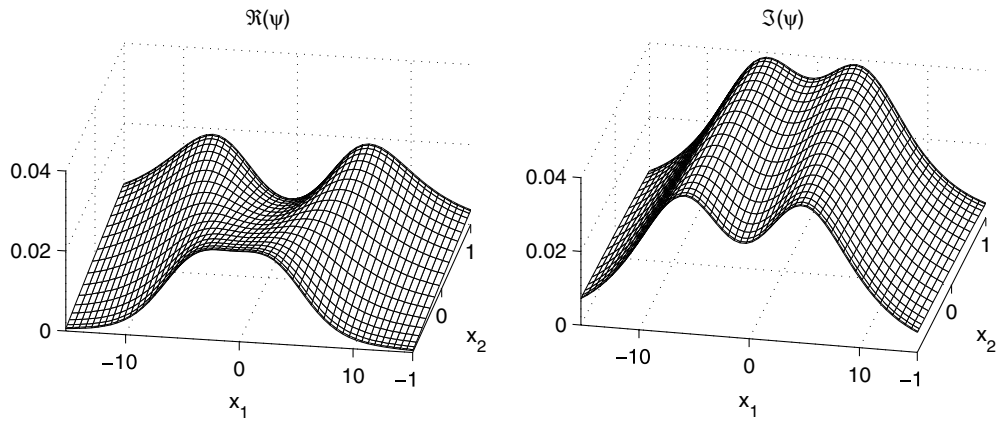
in the continuous spectrum. The behaviour of the other pair of complexified eigenvalues in the left figure is more difficult in that one of them seems to have the turning point inside the continuous spectrum. Because of the collisions we see that the eigenvalues can actually be degenerate if the  $\mathcal{PT}$  symmetry is broken, providing a positive answer to one of the questions from (Q6).

Let us mention that the behaviour of the eigenvalues in the regime of broken  $\mathcal{PT}$  symmetry exhibits certain similarities with the over-damped phenomena as regards the spectrum of the infinitesimal generator of the semigroup associated with the damped wave equation [10–12]. This indicates the unifying framework of Krein spaces behind these two problems [14, 20].

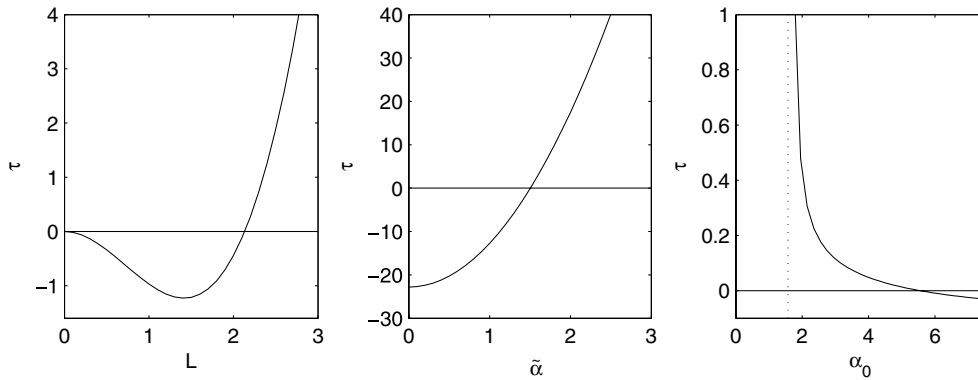
In figure 6, we present an example of eigenfunction corresponding to the case (B1) of theorem 2. We check that the behaviour of the eigenfunction is in perfect agreement with the asymptotic results of theorem 3.

Even if the corresponding eigenenergies are real, the non-Hermiticity prevents from choosing the eigenfunctions real. Since the latter is in particular true for the lowest eigenvalue, it does not make sense to speak about the super- and sub-harmonic properties of the corresponding eigenfunction (which hold in the self-adjoint case). However, although there is no variational characterization of eigenvalues in the present model, numerically we observe that the real and imaginary parts of the eigenfunction corresponding to the lowest eigenvalue are super-harmonic separately in the regime of unbroken  $\mathcal{PT}$  symmetry. This follows, of course, from the observations that they do not change sign and that the spectrum is positive.

Finally, in figure 7, we visualize the dependence of the complicated quantity  $\tau$  defined in (6) on various parameters. In particular, we see that it changes sign, giving a positive answer to (Q1). Consequently, all the cases of theorem 2 for the critical case  $\langle \beta \rangle = 0$  and for the regime  $|\alpha_0| > \pi/d$  can be achieved. We also see that the first figure is in qualitative agreement with an analytic result of ([6], proposition 2.1).



**Figure 6.** Real and imaginary parts of an eigenfunction corresponding to the smallest (positive) eigenvalue of  $H_\alpha$  for  $\alpha(x_1) = 1/3 - 0.65 \exp(-0.025x_1^2)$ .



**Figure 7.** Dependence of  $\tau$  on parameters defining  $\alpha$  in the step-like situation of section 3.1, with  $d = 2$ . The first two figures deal with an antisymmetric square well in the regime  $|\alpha_0| < \pi/d$ , while the last one deals with a symmetric square well in the regime  $\alpha_0 > \pi/d$ . The first (respectively, second) figure shows the dependence of  $\tau$  on the width  $\pm L_\pm =: L$  (respectively, on the coupling  $\tilde{\alpha}$ ) for fixed  $\alpha_0 = 1/3$  and  $\alpha_\pm = \alpha_0 \mp 1$  (respectively, fixed  $\alpha_0 = 1$ ,  $\pm L_\pm = 2$  and variable  $\alpha_\pm = \alpha_0 \mp \tilde{\alpha}$ ). In the last figure, we show the dependence of  $\tau$  on  $\alpha_0$  for  $L = 10$  and variable  $\alpha_\pm = (\alpha_0 - 1)$ ; here the dotted line corresponds to  $\pi/d$ .

### 5. Conclusion

In this paper, we tried to enhance our knowledge of the point spectrum of a non-Hermitian  $\mathcal{PT}$ -symmetric operator introduced in [6] by analysing it numerically. We confirmed theoretical results obtained in [6] by perturbation methods, and showed that they actually hold under much milder conditions about  $\alpha$ .

Besides this, it turned out that the operator can model a fairly wide range of situations. Indeed, its spectrum is very rich, and certain properties we found are unusual when we compare them with the standard self-adjoint cases. Among them we would like to point out the non-monotonic dependence on the strength of perturbation and the existence of the regime

of broken  $\mathcal{PT}$  symmetry. We hope that this study will stimulate further theoretical endeavour to extract and prove the salient features.

In particular, based on the present numerical analysis, we conjecture that there will be no other spectrum except for the continuous one if the parameter  $\varepsilon$  is sufficiently large. At the same time, we were not able to find any discrete eigenvalues in the case of corollary 1, i.e. (Q3) from the end of section 2 seems to have a negative answer; the statement (v) of theorem 1 would be trivial, then. Our numerical experiments also indicate that the condition mentioning in (Q2) is indeed just a technical hypothesis in theorem 2C, in the sense that it does not influence the existence/non-existence of weakly-coupled eigenvalues.

More generally, the existence of eigenvalues in the present model seems to have a nice heuristic explanation. We observe that the discrete spectrum behaves in many respects as that of a one-dimensional Schrödinger operator governed by the first-transverse-eigenvalue potential, i.e.,  $-\Delta + \min\{\alpha^2, \pi^2/d^2\}$  in  $L^2(\mathbb{R})$ . Of course, this self-adjoint idealization is just approximative and cannot explain, in particular, the existence of non-real eigenvalues. However, it provides an insight into the non-monotonicity behaviour, the absence of point spectrum for large  $\varepsilon$ , the positivity of (the real part of) the spectrum, etc. It also formally explains the condition from the statement 1 (respectively, 2) of theorem 2B, since this actually implies that the potential is attractive (respectively, repulsive).

In this paper, we were mainly interested in the eigenvalues emerging from the threshold  $\mu_0^2$  of the continuous spectrum. A complete answer to the first question of (Q7) can be provided by a perturbation method similar to that of [6]. However, a more detailed analysis of the continuous spectrum would be still desirable. In particular, figure 4 suggests that there can be embedded eigenvalues for larger values of the coupling parameter.

Finally, let us point out that the question of a direct physical motivation for the Hamiltonian  $H_\alpha$  remains open. In this paper, we were rather interested in consequences of the non-self-adjointness on spectral properties of this specific model in the context of  $\mathcal{PT}$ -symmetric quantum mechanics. On the other hand, motivated by problems in semiconductor physics, similar self-adjoint, respectively, non-self-adjoint but dissipative, Robin-type boundary conditions have been considered recently in [15], respectively in [16]. In a different context, the present ( $\mathcal{PT}$ -symmetric) Robin-type boundary conditions imply that we actually deal with the Helmholtz equation in an electromagnetic waveguide with radiation/dissipative boundary conditions.

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