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ON THE DISCRETE SPECTRUM OF A WINDOW-COUPLED QUANTUM WAVEGUIDE WITH MIXED BOUNDARY CONDITIONS

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ABSTRACT. In this paper, the discrete spectrum of a straight quantum waveguide with Dirichlet and Robin boundary conditions imposed on different parts of the boundary and a Neumann window is investigated. We prove results on the existence of the discrete spectrum when the Robin parameter is nonnegative. In addition, a lower bound to the distance between the bottom of the essential spectrum and the spectral threshold in terms of the length of the Neumann window is derived.

Keywords. Discrete spectrum, Existence, Quantum waveguide, Spectral threshold

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1. Introduction

In the development of modern technology, guided motion of quantum particles in nanostructures has many useful applications. Quantum waveguides are one of those structures in electron transport with interesting effects that require theoretical attention, see e.g., [3].

Mathematically speaking, maintaining a particle inside a waveguide is made possible through the introduction of Dirichlet, Neumann or Robin conditions or a combination of them at the boundary. The presence of such boundary conditions induces a nontrivial spectrum below the bottom of the essential spectrum consisting of isolated eigenvalues of finite multiplicity, called bound states.

Straight and curved quantum waveguides with different boundary conditions have been studied, and both qualitative and quantitative spectral properties of bound states in these structures analytically stated [2, 7, 10, 11, 13, 15]. Some of these results have been extended to different configurations including two waveguides coupled by a window [5, 6] and waveguides in magnetic fields [16, 18]. More recent literature on the spectral properties of quantum waveguides can be found in [1, 4, 12, 17]. In the present paper, the discrete spectrum of a quantum waveguide with mixed Dirichlet- Robin boundary conditions and a window characterized by

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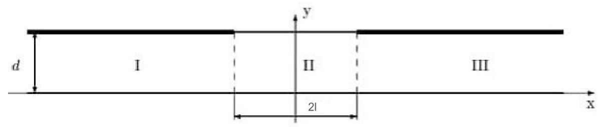

FIGURE 1.

Neumann conditions is studied. Window coupled waveguide models, like the one discussed in this paper, have wide applications in computer science, for example, in optical computing where photons are used to perform computations which offers numerous advantages like faster processing speeds and higher bandwidth. In particular, they are used in devices like arrayed waveguide gratings which are important in wavelength division multiplexing systems [8, 14].

The rest of this paper is organized as follows: In section 2, we present the eigenvalue problem under study, in section 3.1, results on the existence of the discrete spectrum are given and section 3.2 provides a bound on the spectral threshold.

2. The Model

We consider a quantum particle whose motion is guided inside an infinite straight strip of constant width d. One part of the boundary, Dirichlet conditions are imposed while Robin conditions are imposed on the other part (represented by thick and thin lines respectively in figure 1) and a Neumann window of length $2l$ is introduced as described below.

We denote the configuration space by $\Omega := \mathbb{R} \times (0, d)$ and its different parts by $\Omega_I := (-\infty, -l) \times (0, d)$, $\Omega_{II} := (-l, l) \times (0, d)$, $\Omega_{III} := (l, -\infty) \times (0, d)$. The model is given by the following eigenvalue problem for a lower semi-bounded self-adjoint Laplace operator

$$-\Delta u = \lambda u \quad \text{in} \quad \Omega \tag{2.1}$$

on $L^2(\Omega)$ with boundary conditions

$$u_y(x, 0) + \alpha u(x, 0) = 0,\ u(x, d) = 0 \quad \text{on } \partial\Omega_I, \tag{2.2}$$

$$u_y(x, 0) = 0,\ u_y(x, d) = 0 \quad \text{on } \partial\Omega_{II}, \tag{2.3}$$

$$u_y(x, 0) + \alpha u(x, 0) = 0,\ u(x, d) = 0 \quad \text{on } \partial\Omega_{III}, \tag{2.4}$$

where u_y denotes the partial derivative of u with respect to y.

The quadratic form of the operator in (2.1) subject to the boundary conditions in (2.3), (2.2) and (2.4) is given by

$$q_0[u] = \int_\Omega |\nabla u|^2\, dx dy - \alpha \int_A |u(x, 0)|^2\, dx \tag{2.5}$$

with domain

$$D(q_0) = \{u \in \mathcal{H}^1(\Omega) \,:\, u\backslash_D = 0\},$$

where $\mathcal{H}^1(\Omega)$ is the standard Sobolev space, $A := (-\infty, -l) \cup (l, \infty)$ and $u\backslash_D$ denotes the trace of u on the part of the boundary D, where Dirichlet conditions are imposed.

If λ_1 is the first eigenvalue of the self-adjoint one-dimensional Laplacian on $L^2(0, d)$ with the same boundary conditions, the essential spectrum of the operator in (2.1) is the interval $[\lambda_1, \infty)$. The presence of the boundary conditions is expected to induce a nontrivial spectrum in the interval $(-\infty, \lambda_1)$, called the discrete spectrum [3, 7, 10]. When $\alpha = 0$, we have Neumann conditions on the lower boundary outside the window, and in this case, $\lambda_1 = \frac{\pi^2}{4d^2}$, while the case $|\alpha| \longrightarrow \infty$ gives Dirichlet conditions on both sides of the boundary outside the window, and in this case $\lambda_1 = \frac{\pi^2}{d^2}$ [10].

In all our results, the proofs concerning the existence of the discrete spectrum and the bound on the spectral threshold are based on the variational principle, by construction of suitable trial functions following the idea in [9].

3. Main Results

3.1. Existence of the discrete spectrum.

Theorem 3.1. *For any $\alpha \geq 0$, the discrete spectrum of the operator associated with the quadratic form in (2.5) is nonempty.*

Proof. By the variational principle, we look for a trial function $\phi \in D(q_0)$ such that

$$q[\phi] = q_0[\phi] - \lambda_1 \|\phi\|^2 < 0. \tag{3.1}$$

The function ϕ can be chosen continuous in Ω but not necessarily smooth. Let η be the eigenfunction corresponding to λ_1 normalized in $L^2(0, d)$. Let

$$\phi(x, y) = \varphi(x)\eta(y)$$

where $\varphi \in C_0^\infty(\mathbb{R})$ such that $\varphi(x) = 1$ for all $x \in [-l, l]$.
Let $\{\varphi_\sigma \,:\, \sigma > 0\}$ be a family functions given by

$$\varphi_\sigma(x) = \begin{cases} \varphi(x) & \text{if } x \in [-l, l], \\ \varphi(-l + \sigma(x + l)) & \text{if } x \in (-\infty, -l], \\ \varphi(l + \sigma(x - l)) & \text{if } x \in [l, \infty). \end{cases}$$

Furthermore, choose a localization function $j \in C_0^\infty(-l, l)$ and for $\epsilon > 0$, define

$$\begin{aligned} \phi_{\sigma,\epsilon}(x, y) &= \varphi_\sigma(x)(\eta(y) + \epsilon j(x)^2) \\ &= \phi_{1,\sigma,\epsilon} + \phi_{2,\sigma,\epsilon}, \end{aligned} \tag{3.2}$$

where

$$\phi_{1,\sigma,\epsilon} = \varphi_\sigma(x)\eta(y) \text{ and } \phi_{2,\sigma,\epsilon} = \varphi_\sigma(x)\epsilon j(x)^2.$$

The construction has been done by modifying the factorized function ϕ in the mutually disjoint regions Ω_I, Ω_{II} and Ω_{III} so that φ'_σ and j have disjoint supports. We have chosen $\varphi(-l) = \varphi(l)$ since the ground state is expected to be symmetric. We can also assume that the functions φ and j are real-valued. It follows by (2.5) and (3.1) that

$$q[\phi_{\sigma,\epsilon}] = q_0[\phi_{1,\sigma,\epsilon} + \phi_{2,\sigma,\epsilon}] - \lambda_1 \|\phi_{1,\sigma,\epsilon} + \phi_{2,\sigma,\epsilon}\|^2 \tag{3.3}$$

Now, using the properties of η and j, the definition of set A in (2.5) and the fact that the functions φ'_σ and j have disjoint supports, we have

$$\begin{aligned} q_0[\phi_{1,\sigma,\epsilon} + \phi_{2,\sigma,\epsilon}] &= \int_{\mathbb{R}} |\varphi'_\sigma(x)|^2 dx + 4\epsilon^2 d \int_{\mathbb{R}} |\varphi_\sigma(x) j(x) j'(x)|^2 dx \\ &+ \int_{\mathbb{R}} |\varphi_\sigma(x)|^2 dx \int_0^d |\eta'(y)|^2 dy - \alpha\eta(0)^2 \int_A |\varphi_\sigma(x)|^2 dx \\ &= \|\varphi'_\sigma\|^2_{L^2(\mathbb{R})} + 4\epsilon^2 d \|jj'\|^2_{L^2(\mathbb{R})} + \lambda_1 \|\varphi_\sigma\|^2_{L^2(\mathbb{R})} \\ &- \alpha \|\varphi_\sigma\|^2_{L^2(\mathbb{R})} - \alpha\eta(0)^2 \|\varphi_\sigma\|^2_{L^2(A)}, \end{aligned} \tag{3.4}$$

$$\begin{aligned} \|\phi_{1,\sigma,\epsilon} + \phi_{2,\sigma,\epsilon}\|^2 &= \int_{\mathbb{R}} |\varphi_\sigma(x)|^2 dx + 2\epsilon \int_{\mathbb{R}} |j(x)|^2 dx \int_0^d |\eta(y)| dy \\ &+ \epsilon^2 d \int_{\mathbb{R}} |j(x)^2|^2 dx \\ &= \|\varphi_\sigma\|^2_{L^2(\mathbb{R})} + 2\epsilon \|j\|^2_{L^2(\mathbb{R})} \|\eta\|_{L^1(0,d)} + \epsilon^2 d \|j^2\|^2_{L^2(\mathbb{R})} \end{aligned} \tag{3.5}$$

and

$$\begin{aligned} \|\varphi'_\sigma\|^2_{L^2(\mathbb{R})} &= \int_{-\infty}^{-l} \sigma^2 |\varphi'(-l + \sigma(x+l))|^2 dx + \int_l^\infty \sigma^2 |\varphi'(l + \sigma(x-l))|^2 dx \\ &= \sigma^2 \int_A \frac{1}{\sigma} |\varphi'(s)|^2 \, ds \\ &= \sigma \|\varphi'\|^2_{L^2(A)}. \end{aligned} \tag{3.6}$$

Putting (3.4), (3.5) and (3.6) in (3.3) gives

$$\begin{aligned} q[\phi_{\sigma,\epsilon}] &= \sigma \|\varphi'\|^2_{L^2(A)} + \epsilon^2 \left(4d \|jj'\|^2_{L^2(\mathbb{R})} - \lambda_1 d \|j^2\|^2_{L^2(\mathbb{R})} \right) \\ &- 2\lambda_1 \epsilon \|j\|^2_{L^2(\mathbb{R})} \|\eta\|_{L^1(0,d)} - \alpha\eta(0)^2 \|\varphi_\sigma\|^2_{L^2(A)}. \end{aligned} \tag{3.7}$$

Notice that the last three terms do not depend on σ. Moreover, the linear term in ϵ is negative, so one can choose ϵ sufficiently small so that the linear term dominates the quadratic one. Finally, fixing ϵ and choosing σ sufficiently small, the right hand side of (3.7) becomes negative. This concludes the proof. □

3.2. **Estimate for the spectral threshold.** The result in this subsection gives a quantitative measure of the gap between the infimum of the spectrum and the bottom of the essential spectrum. The estimating constant is shown to depend on the length of the Neumann window.

Theorem 3.2. *Let T be the self-adjoint operator associated with (2.5). Then for any $\alpha \geq 0$*

$$\inf \sigma(T) \leq \lambda_1 - \frac{4}{3l^2}. \tag{3.8}$$

Proof. It follows from the variational principle that

$$\inf \sigma(T) - \lambda_1 = \inf_{\psi \in D(q)} \frac{q[\psi]}{\|\psi\|^2_{l^2(\Omega)}} \leq \inf_{\psi \in \mathcal{B}} \frac{q[\psi]}{\|\psi\|^2_{l^2(\Omega)}}, \tag{3.9}$$

where $\mathcal{B}$ is an arbitrary subset of $D(q)$. Our main goal is to a find a suitable subset $\mathcal{B} \subset D(q)$ and explicitly compute the infimum of the quotient in the right hand side of (3.9).
Let

$$\psi_{n,c}(x,y) = \varphi_c(x;n)\eta(y)$$

be the trial function from the domain of q, where η is the normalized eigenfunction corresponding to λ_1 and $\varphi_c(x;n)$ is a mollifier given by

$$\varphi_c(x;n) = \begin{cases} 1 & \text{if } x \in (-n,n), \\ \frac{cn+x}{n(c-1)} & \text{if } x \in (-cn,-n], \\ \frac{cn-x}{n(c-1)} & \text{if } x \in [n,cn), \\ 0 & \quad \text{elsewhere }, \end{cases}$$

where $c > 1$. Set

$$\mathcal{B} := \{\psi_{n,c} \in D(q) \,:\, n \geq l,\, c > 1\}.$$

Then

$$\begin{aligned} q[\psi_{n,c}] &= \int_{\mathbb{R}} |\varphi_c'(x;n)|^2 dx + \lambda_1 \int_{\mathbb{R}} |\varphi_c(x;n)|^2 dx - \alpha\eta(0)^2 \int_{\mathbb{R}} |\varphi_c(x;n)|^2 dx \\ &- \alpha\eta(0)^2 \int_A |\varphi_c(x;n)|^2 dx - \lambda_1 \int_{\mathbb{R}} |\varphi_c(x;n)|^2 dx \\ &\leq \|\varphi'(x;n)\|^2_{L^2(\mathbb{R})} \\ &= \frac{2}{n(c-1)}, \end{aligned} \tag{3.10}$$

$$\begin{aligned} \|\psi_{n,c}\|^2_{L^2(\Omega)} &= \int_{\mathbb{R}} |\varphi_c(x;n)|^2 dx \int_0^d |\eta(y)|^2 dy \\ &= \int_{-cn}^{-n} |\frac{cn+x}{n(c-1)}|^2 dx + 2n + \int_n^{cn} |\frac{cn-x}{n(c-1)}|^2 dx \\ &= \frac{2n(c^3-3c+2)}{3(c-1)^2}. \end{aligned} \tag{3.11}$$

It follows by (3.10) and (3.11) that

$$\frac{q[\psi_{n,c}]}{\|\psi_{n,c}\|^2_{L^2(\Omega)}} \leq \frac{3(c-1)}{n^2(c^3-3c+2)}. \tag{3.12}$$

Let $\Omega_0 := (l, \infty) \times (1, \infty)$ and set

$$g(n, c) = \frac{3(c-1)}{n^2(c^3 - 3c + 2)}.$$

Since for all $(n, c) \in \Omega_0$, $\frac{\partial g}{\partial n} \neq 0$ and $\frac{\partial g}{\partial c} \neq 0$, then one can easily see that g has no local minimum inside Ω_0. Therefore, we study the behaviour of the function along the boundary $\{l\} \times (1, \infty)$ and its limits as $c \longrightarrow 1$ and $c \longrightarrow \infty$ respectively. Notice that $g(n, c) \geq 0$ inside Ω_0 and the function $g(l, .)$ achieves its local negative minimum

$$g\left(l, -\frac{1}{2}\right) = -\frac{4}{3l^2}.$$

Hence there is a finite $n_0 \geq l$ such that for every $n \geq n_0$

$$g(n, c) \geq -\frac{4}{3l^2}.$$

So, it is sufficient to find the minimum of g for only those values of $n \in [l, n_0]$. However, all $n \in [l, n_0]$

$$g(n, c) \geq \frac{3}{n_0^2(c-1)(c+2)}.$$

Since

$$\lim_{c \longrightarrow 1} \frac{3}{n_0^2(c-1)(c+2)} = \infty \text{ and } \lim_{c \longrightarrow \infty} \frac{3}{n_0^2(c-1)(c+2)} = 0,$$

then, we have

$$\lim_{c \longrightarrow \infty} \inf g(n, c) \geq 0.$$

Again, since $g(l, -\frac{1}{2}) < 0$, then, one has

$$\inf_{(n,c) \in \Omega_0} g(n, c) = \inf_{c \in (1, \infty)} g(n, c) = -\frac{4}{3l^2}.$$

Hence, (3.8) follows from (3.9) and (3.12). $\square$

Remark 3.3. The estimating constant in (3.8) is independent of the width of the waveguide, and so, it is expected to hold for straight waveguides of any width. Moreover, the estimate in (3.8) implies that for waveguides with very large values of l, $\inf \sigma(T) \leq \lambda_1$, and for waveguides with very small windows $\inf \sigma(T) = -\infty$. Therefore, it is nontrivial to ask for the interval (l_0, l_1) for which there is constant $C(l) > 0$ and

$$\inf \sigma(T) \leq \lambda_1 - C(l), \;\; l \in (l_0, l_1).$$

In addition, it is also important to study the asymptotic behaviour of the estimate in the limit as $l \longrightarrow l_0$ or $l \longrightarrow l_1$ (cf. [2]).

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