Bound states in a locally deformed waveguide: the critical case

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Abstract. We consider the Dirichlet Laplacian for a strip in $\mathbb{R}^2$ with one straight boundary and a width $a(1+\lambda f(x))$, where f is a smooth function of a compact support with a length $2b$. We show that in the critical case, $\int_{-b}^{b} f(x)\,dx = 0$, the operator has no bound states for small $|\lambda|$ if $b < (\sqrt{3}/4)a$. On the other hand, a weakly bound state exists provided $\|f'\| < 1.56a^{-1}\|f\|$; in that case there are positive c_1, c_2 such that the corresponding eigenvalue satisfies $-c_1\lambda^4 \le \epsilon(\lambda) - (\pi/a)^2 \le -c_2\lambda^4$ for all $|\lambda|$ sufficiently small.

1 Introduction

Quantum waveguides, *i.e.*, systems in which a quantum mechanical particle is confined to a tubular region, attracted a wave of attention induced by the progress of the "mesoscopic" physics — some reference and a guide to further reading can be found in [DE, DES]. Apart of a natural physical interest, some interesting mathematical problems arose in this connection.

One of them concerns the existence of bound states which appear if a Dirichlet tube of a constant cross section is locally deformed, *e.g.*, bent — see [ES, DE] and references therein. Another mechanism producing bound states in straight tubes is based on tube protrusions [ISY, AS]. It has been treated rigorously in a recent paper by Bulla et al. [BGRS] where the asymptotic behavior of the eigenvalue for a gentle deformation was found.

In distinction to bent tubes a local variation of the cross section can yield both an attractive and repulsive effective interaction; it is easy to see that constrictions produce no bound states. A more subtle question is what happens if the profile modification along the tube includes both an expansion and squeezing. It is demonstrated in [BGRS] that the "averaged" cross–section variation matters: a bound state exists in a slightly deformed tube provided the added volume is positive while in the opposite case it is absent. In the former case, the asymptotic behavior of the gap is governed by the square of the deformation parameter λ.

In this letter we address the critical case left out in the mentioned paper, namely the situation when the volume change is zero. The authors pointed out that bound states might exist in view of the analogy with one–dimensional Schrödinger operators [BGS, Si, Kl], however, they remarked at the same time that the effect of the additional second–order terms in the Hamiltonian is not apriori obvious. For the sake of simplicity we restrict ourselves to the basic setup of [BGRS]: we consider a planar strip obtained be deforming locally *one* boundary of $\Omega_0 := I\!\!R \times [0,a]$. We show that the answer depends on the shape of the deformation. If the latter is localized into an interval sufficiently small with respect to tube width a, there is no bound state. On the other hand, a bound state exists if the deformation is smeared enough, and the leading behavior of the gap is given in this case by the *fourth* power of the parameter λ.

2 The results

We consider the Dirichlet Laplacian $-\Delta^D_{\Omega_\lambda}$ on a deformed strip

$$\Omega_\lambda := \{\, (x,y) \in I\!\!R^2 :\ 0 < y < a(1+\lambda f(x))\,\}\,, \tag{1}$$

where $f \in C_0^\infty(I\!\!R)$ is a given function; in distinction to [BGRS] we do not put $a=1$. Our main results are the following:

Theorem 1 *Suppose that* $f \in C_0^\infty(I\!\!R)$ *is such that* $\operatorname{supp} f \subset [-b,b]$ *and*

$$\int_{-b}^{b} f(x)\, dx \;=\; 0\,; \tag{2}$$

then the discrete spectrum of $-\Delta^D_{\Omega_\lambda}$ *is empty for all sufficiently small* $|\lambda|$ *provided*

$$a \;>\; \frac{4}{\sqrt{3}}\, b\,. \tag{3}$$

Theorem 2 *Under the same assumptions,* $-\Delta^D_{\Omega_\lambda}$ *has an isolated eigenvalue* $\epsilon(\lambda)$ *for any nonzero* λ *with* $|\lambda|$ *small enough provided*

$$\frac{\|f'\|^2}{\|f\|^2} \;<\; \left(\frac{\pi}{a}\right)^2 \frac{6}{9+\sqrt{90+12\pi^2}}\,. \tag{4}$$

In that case there are positive $c_1,\, c_2$ *such that*

$$-c_1\lambda^4 \;\le\; \epsilon(\lambda) - \left(\frac{\pi}{a}\right)^2 \;\le\; -c_2\lambda^4\,. \tag{5}$$

3 Nonexistence of bound states

By [BGRS], the operator under consideration is unitarily equivalent to

$$H_\lambda = -\Delta^D_{\Omega_0} + \lambda A_1 - \lambda^2 A_2 \tag{6}$$

on $L^2(\Omega_0)$ corresponding to the straightened strip $\Omega_0 := I\!R \times [0,a]$, where

$$A_1 = \sum_{j=1}^{5} A_{1j}\,, \qquad A_2 = \sum_{j=1}^{6} A_{2j}$$

with

$$\begin{aligned} &A_{11} = 2f(x)\partial_y^2\,, \quad A_{12} = yf''(x)\partial_y\,, \quad A_{13} = 2yf'(x)\partial^2_{xy}\,, \\ &A_{14} = f'(x)\partial_x\,, \quad A_{15} = \frac{1}{2}\,f''(x)\,, \end{aligned} \tag{7}$$

and

$$\begin{aligned} A_{21} &= \frac{3f(x)^2 + 2\lambda f(x)^3 + y^2 f'(x)^2}{(1+\lambda f(x))^2}\,\partial_y^2\,, \quad A_{22} = \left(\frac{yf(x)f''(x)}{1+\lambda f(x)} + \frac{3yf'(x)^2}{(1+\lambda f(x))^2}\right)\partial_y\,, \\ A_{23} &= \frac{2yf(x)f'(x)}{1+\lambda f(x)}\,\partial^2_{xy}\,, \qquad A_{24} = \frac{f(x)f'(x)}{1+\lambda f(x)}\,\partial_x\,, \\ A_{25} &= \frac{f(x)f'(x)}{2(1+\lambda f(x))}\,, \qquad A_{26} = \frac{3f'(x)^2}{4(1+\lambda f(x))^2}\,. \end{aligned} \tag{8}$$

Since $\inf \sigma_{ess}(H_\lambda) = (\pi/a)^2$, Theorem 1 will be proven if we demonstrate that $(H_\lambda\psi,\psi) \ge (\pi/a)^2$ holds for all ψ from a suitable dense set, say, $C_0^2(\Omega_0)$. Such a function can be always written as

$$\psi(x,y) = G(x,y) + R(x,y)\,, \tag{9}$$

where $G(x,y) = \phi(x)\chi_1(y)$ and $R(x,\cdot) \perp \chi_1$ for all $x \in I\!R$; we use the symbol χ_n for the normalized n–th transverse–mode eigenfunction,

$$\chi_n(y) := \sqrt{\frac{2}{a}}\,\sin\left(\frac{\pi n y}{a}\right)\,. \tag{10}$$

The smooth function ϕ can be written as $\phi(x) = \alpha + g(x)$, where $\alpha := \phi(-b)$. In view of (6), the quadratic form to be estimated can be expressed as

$$\begin{aligned} (H_\lambda\psi,\psi) = &-(\Delta^D_{\Omega_0}G,G) - (\Delta^D_{\Omega_0}R,R) \\ &+\lambda(A_1G,G) + \lambda(A_1R,R) + 2\lambda\,\mathrm{Re}\,(A_1G,R) \\ &-\lambda^2(A_2G,G) - \lambda^2(A_2R,R) - 2\lambda^2\mathrm{Re}\,(A_2G,R)\,. \end{aligned} \tag{11}$$

Let us begin with the terms linear in λ. With an abuse of notation, $A_1(1\times\chi_1)=A_1\chi_1$, we write

$$(A_1G,G)\;=\;\alpha^2(A_1\chi_1,\chi_1)+\alpha(A_1\chi_1,g\chi_1)+(A_1g\chi_1,g\chi_1)\,.$$

The first term at the *rhs* is zero in view of (2) and $\int_{-b}^{b}f''(x)\,dx=f'(b)-f'(-b)=0$. The second one is

$$-2\alpha\left(\frac{\pi}{a}\right)^2(f,g)_{L^2(-b,b)}-\frac{\alpha}{2}(f',g')_{L^2(-b,b)}-\alpha(y\chi_1',\chi_1)_{L^2(0,a)}(f',g')_{L^2(-b,b)}\,,$$

where we have used integration by parts together with $-\chi_1''=(\pi/a)^2\chi_1$; evaluating the inner product we see that the last two terms cancel. Finally, using the fact that f,f',f'' are bounded on $[-b,b]$, we arrive at the bound

$$|(A_1g\chi_1,g\chi_1)|\;\le\;C\left(\|g\|^2_{L^2(-b,b)}+\|g'\|^2_{L^2(-b,b)}\right)\;;$$

here and in the following C is an unspecified positive constant which assume different values in different expressions. In fact, the derivative norm alone may be used here, because $g(-b)=0$ implies easily

$$\|g\|^2_{L^2(-b,b)}\;\le\;(2b)^2\|g'\|^2_{L^2(-b,b)}\,. \tag{12}$$

Together we have

$$\lambda(A_1G,G)\;\ge\;-2\alpha\left(\frac{\pi}{a}\right)^2(f,g)_{L^2(-b,b)}-\lambda C\|g'\|^2_{L^2(-b,b)}\,.$$

In a similar way the boundedness of f,f',f'' together with integration by parts and the Schwarz inequality yield

$$|(A_1R,R)|\;\le\;C\|R\|^2_{W_2^1(\Omega_b)}\,,$$

where $\Omega_b:=[-b,b]\times[0,a]$. The same argument applies to the "α–indepedent part" of the mixed term,

$$|(A_1g\chi_1,R)|\;\le\;C\left(\|g'\|^2_{L^2(-b,b)}+\|R\|^2_{L^2(\Omega_b)}\right)\,.$$

The remaining term needs more attention. Since R is smooth by assumption, it may be represented pointwise as

$$R(x,y)\;=\;\sum_{n=2}^{\infty}r_n(x)\chi_n(y)\,, \tag{13}$$

so

$$\alpha(A_1\chi_1,R)\;=\;-\alpha\sum_{n=2}^{\infty}(f',g')_{L^2(-b,b)}(y\chi_1',\chi_n)_{L^2(0,a)}\,. \tag{14}$$

The last inner product equals $(-1)^n 2n/(n^2-1)$; we introduce

$$K := \left(\sum_{n=2}^{\infty} \left(\frac{2n}{n^2-1} \right)^2 \right)^{1/2} . \tag{15}$$

The last sum can be evaluated [PBM, Sec. 5.1] in terms of the di– and trigamma functions ψ and ψ', respectively, as

$$4 \sum_{n=1}^{\infty} \frac{(n+1)^2}{n^2(n+2)^2} = \pi^2 - \frac{31}{4} + 2(\psi(3)+\gamma) - 4\psi'(3) \,,$$

and since $2(\psi(3)+\gamma) = 3$ and $4\psi'(3) = 4\zeta(2)-5$ by [AbS, Chap. 6], where ζ is the Riemann zeta function and γ is the Euler's constant, we obtain

$$K = \sqrt{\frac{\pi^2}{3} + \frac{1}{4}} . \tag{16}$$

The term (14) in question may be then estimated in modulus by

$$\alpha \left(|f'|, \sum_{n=2}^{\infty} |r_n'| \frac{2n}{n^2-1} \right)_{L^2(-b,b)} \le \alpha K \left(|f'|, \left(\sum_{n=2}^{\infty} |r_n'|^2 \right)^{1/2} \right)_{L^2(-b,b)}$$

$$\le \frac{1}{2}\, \alpha^2 K^2 \lambda (1+\tilde{c}\lambda) \|f'\|^2_{L^2(-b,b)} + \frac{1}{2\lambda(1+\tilde{c}\lambda)} \|R_x\|^2_{L^2(\Omega_b)} \,,$$

where $R_x := \partial R/\partial x$ and $\tilde{c}$ is a positive number to be specified later; in the last step we have used the Schwarz inequality.

Next, we pass to the quadratic terms. By the boundedness of f, f', f'' we have

$$\lambda^2 |(A_2 R, R)| \le C\lambda^2 \|R\|^2_{W_2^1(\Omega_b)} \,;$$

the same property in combination with the Schwarz inequality and the estimate (12) gives for the two parts of the mixed term

$$\lambda^2 \alpha |(A_2 \chi_1, R)| \le C\alpha^2 \lambda^3 + \frac{\lambda}{2} \|R\|^2_{L^2(\Omega_b)}$$

$$\lambda^2 |(A_2 g \chi_1, R)| \le C\lambda^3 \|g'\|^2_{L^2(-b,b)} + \frac{\lambda}{2} \|R\|^2_{L^2(\Omega_b)} \,.$$

The remaining quadratic term which refers to the lowest transverse–mode component equals

$$\lambda^2 \Big(\alpha^2 (A_2 \chi_1, \chi_1) + 2\alpha \,\mathrm{Re}\, (A_2 g \chi_1, \chi_1) + (A_2 g \chi_1, g \chi_1) \Big) \,.$$

The last two terms at the *rhs* are estimated as above

$$\lambda^2 \alpha |(A_2 g \chi_1, g \chi_1)| \le C\lambda^2 \|g'\|^2_{L^2(-b,b)}$$

$$\lambda^2 |(A_2 \chi_1, g \chi_1)| \le C\alpha^2 \lambda^3 + \frac{\lambda}{2} \|g\|^2_{L^2(-b,b)} \,,$$

while the first one can be evaluated from

$$(A_2\chi_1,\chi_1) \;=\; -3\left(\frac{\pi}{a}\right)^2 \|f\|^2_{L^2(-b,b)} - \left(\frac{\pi}{a}\right)^2 \|f'\|^2_{L^2(-b,b)} (y^2\chi_1,\chi_1)_{L^2(0,a)}$$

$$+2\|f'\|^2_{L^2(-b,b)}(y\chi_1',\chi_1)_{L^2(0,a)} + \frac{1}{4}\|f'\|^2_{L^2(-b,b)} + \mathcal{O}(\lambda)\,.$$

Computing the inner products and using (16), we arrive thus at the expression

$$\lambda^2(A_2\chi_1,\chi_1) \;=\; -\lambda^2\alpha^2\left(3\left(\frac{\pi}{a}\right)^2 \|f\|^2_{L^2(-b,b)} + K^2\|f'\|^2_{L^2(-b,b)}\right) + \mathcal{O}(\lambda^3)\,.$$

Putting the results obtained up to now together, we find for the *rhs* of (11) the bound

$$\begin{aligned}(H_\lambda\psi,\psi) \;\geq\; & \|\nabla G\|^2 + \|\nabla R\|^2 + 3\lambda^2\alpha^2\left(\frac{\pi}{a}\right)^2 \|f'\|^2_{L^2(-b,b)} - 2\lambda\alpha\left(\frac{\pi}{a}\right)^2 (f,g)_{L^2(-b,b)} \\ & -(1+\tilde{c}\lambda)^{-1}\|R_x\|^2_{L^2(\Omega_b)} - C\left(\lambda\|g'\|^2_{L^2(-b,b)} + \lambda\|R\|^2_{W_2^1(\Omega_b)} + \alpha^2\lambda^3\right)\,,\end{aligned} \tag{17}$$

which is valid for all $|\lambda|$ small enough. It remains to estimate the "kinetic" terms. Using once more the decomposition (13), we derive

$$\|\nabla R\|^2 \;\geq\; \|R_x\|^2_{L^2(\Omega_b)} + \left(\frac{2\pi}{a}\right)^2 \|R\|^2_{L^2(\Omega_b)}\;;$$

the inequality

$$\|\nabla R\|^2 - \lambda C\|R\|^2_{W_2^1(\Omega_b)} - (1+\tilde{c}\lambda)^{-1}\|R_x\|^2_{L^2(\Omega_b)} \;\geq\; \left(\frac{2\pi}{a}\right)^2 \|R\|^2_{L^2(\Omega_b)}$$

is then satisfied if

$$\frac{\tilde{c}-C}{1+\tilde{c}\lambda} \;>\; 0 \qquad \text{and} \qquad 3\left(\frac{\pi}{a}\right)^2 - \lambda C \;>\; 0\,,$$

i.e., for $\tilde{c} > C$ and all $|\lambda|$ small enough. In a similar way, we obtain

$$\|\nabla G\|^2 \;\geq\; \|g'\|^2_{L^2(-b,b)} + \left(\frac{\pi}{a}\right)^2 \|G\|^2_{L^2(\Omega_b)}\,.$$

Without loss of generality we may assume $f \neq 0$. We insert the gradient–term estimates into (17) and estimate $\|g'\|^2_{L^2(-b,b)}$ from below by $\|g\|^2_{L^2(-b,b)}$. This can be done by the inequality (12), however, the latter is unnecessarily rough. Minimization of $\|g'\|^2_{L^2(-b,b)}$ for fixed $g(-b)=0$, $g(b)$, and $\|g\|^2_{L^2(-b,b)}$ is an isoperimetric problem [Re, Sec.23F]; the corresponding Euler's equation is easily seen to be solved by a multiple of $\sin\kappa(x-b)$. Taking a minimum over κ, we get

$$\|g'\|^2_{L^2(-b,b)} \;\geq\; \left(\frac{\pi}{4b}\right)^2 \|g\|^2_{L^2(-b,b)}\,. \tag{18}$$

Using this bound, we arrive at

$$(H_\lambda\psi,\psi)-\left(\frac{\pi}{a}\right)^2\|\psi\|^2\;\geq\;\pi^2\,\frac{1-C\lambda}{16b^2}\,\|g\|^2_{L^2(-b,b)}$$

$$-\,2\alpha\lambda\left(\frac{\pi}{a}\right)^2(f,g)_{L^2(-b,b)}+\lambda^2\|f\|^2_{L^2(-b,b)}\left(3\alpha^2\left(\frac{\pi}{a}\right)^2-\frac{C\alpha^2\lambda}{\|f\|^2_{L^2(-b,b)}}\right)\;;$$

the quadratic form at the *rhs* is positive as long as

$$\left(\frac{\pi}{a}\right)^4\;<\;\pi^2\left(\frac{1-C\lambda}{16b^2}\right)\left(3\left(\frac{\pi}{a}\right)^2-\frac{C\lambda}{\|f\|^2_{L^2(-b,b)}}\right)\,. \tag{19}$$

If the inequality is satisfied for $\lambda=0$ the same is true for $|\lambda|$ small enough; this yields the condition (3) and finishes thus the proof of Theorem 1.

4 Existence of bound states

Let us start from a lower bound to possible eigenvalues. A necessary condition for their existence is that the condition (19) is violated. It follows easily from the above estimates that

$$(H_\lambda\psi,\psi)-\left(\frac{\pi}{a}\right)^2\|\psi\|^2\;\geq\;\|G_x\|^2_{L^2(\Omega_b^c)}-\lambda^2\alpha^2 d_0\|f\|^2+\mathcal{O}(\lambda^3)\,, \tag{20}$$

where $\Omega_b^c:=\Omega_0\setminus\Omega_b$ is the complement containing the strip tails, and

$$d_0\;:=\;\left(\frac{4\pi b}{a^2}\right)^2-3\left(\frac{\pi}{a}\right)^2\;;$$

if a bound state exists this quantity has to be positive. Consider a function ψ for which the *lhs* of (20) is negative. We employ the inequality $\|\psi\|^2\geq\|G\|^2_{L^2(\Omega_b^{c,-})}$, where $\Omega_b^{c,-}$ is the left tail, and an analogous bound for $\|G_x\|^2_{L^2(\Omega_b^c)}$. The functional

$$\mathcal{L}(G)\;:=\;\frac{\|G_x\|^2_{L^2(\Omega_b^{c,-})}-\lambda^2\alpha^2 d_0\|f\|^2}{\|G\|^2_{L^2(\Omega_b^{c,-})}}\;=\;\frac{\|\phi'\|^2_{L^2(-\infty,-b)}-\lambda^2\alpha^2 d_0\|f\|^2}{\|\phi\|^2_{L^2(-\infty,-b)}}$$

defined on functions with fixed $\phi(-b)=\alpha$ assumes its extremum for $G_0(x,y)=\alpha\,e^{\kappa(x+b)}\chi_1(y)$ with $\kappa=\lambda^2 d_0\|f\|^2$; the minimum value is $-\lambda^4 d_0^2\|f\|^4$. Consequently, we get

$$\frac{(H_\lambda\psi,\psi)}{\|\psi\|^2}-\left(\frac{\pi}{a}\right)^2\;\geq\;-d_0^2\|f\|^4\lambda^4+\mathcal{O}(\lambda^5)\,,$$

i.e., the lower bound (5) of Theorem 2.

The rest of the argument is easier. To check the existence claim of Theorem 2, it is sufficient to use a suitable trial function. We choose

$$\psi_\lambda(x,y) \;=\; (1+\lambda\eta f(x))\chi_1(y)\,, \tag{21}$$

where η is a parameter to be determined; this allows us to employ the above estimates with $R=0$ $\alpha=1$, and $g=\lambda\eta f$. In particular, we have

$$\begin{aligned}(H_\lambda\psi,\psi) \;-\; \left(\frac{\pi}{a}\right)^2\|\psi\|^2 \;&\le\; \|\psi_x\|_{L^2(\Omega_b^c)} \\ &+\; \lambda^2\left\{(3-2\eta)\left(\frac{\pi}{a}\right)^2\|f\|^2+(\eta^2+K^2)\|f'\|^2\right\}+C\lambda^3\,;\end{aligned}$$

since the first term at the *rhs* can be made arbitrarily small, a bound state exists as long as the curly bracket is negative. This condition can be rewritten as

$$\eta^2-2\eta z+3z+K^2\;<\;0\,,\qquad z:=\left(\frac{\pi}{a}\right)^2\frac{\|f\|^2}{\|f'\|^2}\,,$$

so it can be satisfied provided $z^2-3z-K^2>0$, which requires in turn

$$z\;>\;\frac{3+\sqrt{9+4K^2}}{2}\;;$$

substituting for K from (16), we arrive at the condition (4).

It remains to find an upper bound to the eigenvalue $\epsilon(\lambda)$. We put $\eta=z$, so

$$(H_\lambda\psi,\psi)-\left(\frac{\pi}{a}\right)^2\|\psi\|^2 \;=\; \|\psi_x\|_{L^2(\Omega_b^c)}-\lambda^2\|f\|^2d_1+\mathcal{O}(\lambda^3)\,,$$

where $d_1:=\left(\frac{\pi}{a}\right)^2(z-3-z^{-1}K^2)>0$. Outside Ω_b we choose the trial function as follows:

$$\psi(x,y)\;:=\;\left\{\begin{array}{lll} e^{-\kappa|x\mp b|}\chi_1(y) & \dots & \pm x>b \\ \\ 0 & \dots & \text{otherwise}\end{array}\right.$$

where $\kappa=\frac{1}{2}\lambda^2d_1\|f\|^2$. In that case ψ clearly belongs to the form domain of H_λ and

$$\frac{(H_\lambda\psi,\psi)}{\|\psi\|^2}-\left(\frac{\pi}{a}\right)^2\;\le\;\frac{-\frac{1}{2}d_1\|f\|^2\lambda^2}{2b-\frac{2}{\lambda^2d_1\|f\|^2}-C\lambda}\;=\;-\frac{1}{4}d_1^2\|f\|^4\lambda^4+\mathcal{O}(\lambda^5)\,,$$

which yields the other bound of (5).

5 Concluding remarks

The result discussed here is certainly not optimal. To illustrate this, let us ask what is the maximum value of $\frac{a}{b}$ for which the sufficient condition (4) may be satisfied. Since the function f satisfies the condition (2) and $f(b) = 0$, even the inequality (18) cannot be saturated for it; minimizing over the smaller class, we obtain

$$\inf \frac{\|f'\|^2}{\|f\|^2} = \left(\frac{\pi}{b}\right)^2 .$$

Hence examples of critical–tube shapes satisfying the condition (4) exist if

$$\frac{a}{b} < \sqrt{\frac{2}{3+\sqrt{9+4K^2}}} \approx 0.506 \,;$$

on the other hand, the condition (3) excludes the existence of bound states for the ratio $\frac{a}{b} > 2.309$.

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