Asymptotic estimates for bound states in quantum waveguides coupled laterally through a narrow window

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Abstract. Consider the Laplacian in a straight planar strip of width d, with the Neumann boundary condition at a segment of length $2a$ of one of the boundaries, and Dirichlet otherwise. For small enough a this operator has a single eigenvalue $\epsilon(a)$; we show that there are positive c_1, c_2 such that $-c_1 a^4 \le \epsilon(a) - (\pi/d)^2 \le -c_2 a^4$. An analogous conclusion holds for a pair of Dirichlet strips, of generally different widths, with a window of length $2a$ in the common boundary.

1 Introduction

Recent progress in "mesoscopic" physics brought not only new physical effects but also some interesting spectral problems. 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 or protruded, or coupled to another tube — see [BGRS, ES, DE, SRW] and references therein. In this paper we are concerned with another system of this type, which consists of a pair of parallel Dirichlet strips coupled laterally through a window in the common boundary; if they are of the same width the problem simplifies to a treatment of a single strip with the Dirichlet boundary condition changed to Neumann at a segment of the boundary.

Such a window–coupled system represents an idealized setup for some existing quantum–wire devices [HTW, Ku, LS, WG]. Its spectral and scattering properties were discussed in recent papers [BGRS, ESTV]. It was shown there, in particular, that the discrete spectrum was nonempty for any window width $2a > 0$; if the latter is small enough, there is just one simple eigenvalue $\epsilon(a)$ below the bottom of the essential spectrum.

A question naturally arises about the behavior of the gap as $a \to 0$. The result of [BGRS] in combination with a simple bracketing argument shows that it is bounded from below by $c\, a^{4+\varepsilon}$; a numerical analysis performed in [ESTV] suggests that the asymptotic behavior is governed by the fourth power of the window width. Our goal here is to prove two–sided asymptotic estimates of this type.

2 The results

Consider a straight planar strip $\Sigma := I\!\!R \times [-d_2, d_1]$. Given $a > 0$, we denote by $H(d_1, d_2; 2a)$ the Laplacian on $L^2(\Sigma)$ subject to the Dirichlet condition at $y = -d_2, d_1$ as well as at the $|x| > a$ halfline segments of the x–axis; this operator coincides with the Dirichlet Laplacian at the strip with the cuts — see [RS4, Sec.XIII.15]. Set $d := \max\{d_1, d_2\}$. If $d_1 = d_2$, the operator decomposes into an orthogonal sum with respect to the y–parity; the nontrivial part is unitarily equivalent to the Laplacian on $L^2(\Sigma_+)$, where $\Sigma_+ := I\!\!R \times [0, d]$, with the Neumann condition at the segment $[-a, a]$ of the x–axis and Dirichlet at the remaining part of the boundary; we denote it by $H(d; 2a)$.

Basic spectral properties of these operators are the following [BGRS, ESTV]:

Proposition 2.1 $\sigma_{ess}(H(d_1, d_2; 2a)) = [(\pi/d)^2, \infty)$. *The discrete spectrum is nonempty for any $a > 0$ and consists of a finite number of simple eigenvalues $(\pi/D)^2 < \epsilon_1(a) < \ldots \epsilon_N(a) < (\pi/d)^2$, where $D := d_1 + d_2$; if a is small enough there is just one $\epsilon(a) \equiv \epsilon_1(a)$.*

Our main result are asymptotic bounds for the narrow–window case:

Theorem 2.2 *There are positive c_1, c_2 such that*

$$-c_1 a^4 \le \epsilon(a) - \left(\frac{\pi}{d}\right)^2 \le -c_2 a^4 \tag{2.1}$$

holds for all sufficiently small a.

A proof of this theorem is the contents of the following sections.

3 An upper bound

Let us begin with the operator $H \equiv H(d; 2a)$. We denote by $\chi_n(y) = \sqrt{\frac{2}{d}}\, \sin\left(\frac{\pi n y}{d}\right)$, $n = 1, 2, \ldots$, elements of the "transverse" orthonormal basis (the symbol should not be confused with the indicator function χ_M of a set M), and set $\psi = F + G$, where

$$f(x,y) := f_1(x)\chi_1(y)\,, \qquad f_1(y) := \alpha \max\{1,\, e^{-\kappa||x|-a|}\}\,, \tag{3.1}$$

and

$$G(x,y) := \eta\, \chi_{[-a,a]}(x)\, \cos\left(\frac{\pi x}{2a}\right)\, R(y) \tag{3.2}$$

with

$$R(y) := \begin{cases} e^{-\pi y/2a} & \dots \quad y \in \left[0, \frac{d}{2}\right] \\ \\ 2\left(1-\frac{y}{d}\right) e^{-\pi d/4a} & \dots \quad y \in \left[\frac{d}{2}, d\right] \end{cases} \tag{3.3}$$

To make ψ a trial function of $Q(H)$ we have to ensure that it satisfies the Neumann boundary condition at the window, *e.g.*, replacing G by G^ε such that

$$G^\varepsilon(x,d) = 0\,, \qquad G^\varepsilon_y(x,0) = -\,\frac{\sqrt{2}\,\alpha\pi}{d^{3/2}}\,,$$

for $|x| \le a$, where the subscript is a shorthand for the partial derivative, and

$$\max\Big\{\, \|G^\varepsilon - G\|,\ \|\nabla G^\varepsilon - \nabla G\|,\ \|G^\varepsilon(\cdot,0) - G(\cdot,0)\|_{L^2(-a,a)} \,\Big\} < \varepsilon\,.$$

We have to compute $L(\psi^\varepsilon) := (H\psi^\varepsilon, \psi^\varepsilon) - \left(\frac{\pi}{d}\right)^2 \|\psi^\varepsilon\|^2$. The operator part equals $\|\psi^\varepsilon_x\|^2 + \|\psi^\varepsilon_y\|^2$, where the second term is evaluated using $-\chi_1'' = \left(\frac{\pi}{d}\right)^2 \chi_1$, a simple integration by parts, and the explicit value $\chi_1'(0) = \pi\sqrt{2/d^3}$; together we get

$$L(\psi^\varepsilon) \;=\; \|\psi^\varepsilon_x\|^2 + \|G^\varepsilon_y\|^2 - \left(\frac{\pi}{d}\right)^2 \|G^\varepsilon\|^2 - 2\alpha\,\frac{\pi}{d}\sqrt{\frac{2}{d}}\int_{-a}^{a} G^\varepsilon(x,0)\,dx\,. \tag{3.4}$$

It is sufficient to find the *rhs* for ψ since the difference can be made arbitrarily small by a suitable choice of ε.

Since f_x, G_x have disjoint supports, we have $\|\psi_x\|^2 = \|F_x\|^2 + \|G_x\|^2$. Furthermore, the last term equals $\eta^2\,\frac{\pi^2}{4a}\,\|R\|^2_{L^2(0,d)}$, and

$$\|R\|^2_{L^2(0,d)} \;=\; \frac{a}{\pi} + \left(\frac{d}{6} - \frac{a}{\pi}\right) e^{-\pi d/2a} \;<\; \frac{a}{\pi}\,(1+\varepsilon_1)$$

for any $\varepsilon_1 > 0$ and all a small enough. In the same way, $\int_{-a}^{a} G(x,0)\,dx = \frac{4a\eta}{\pi}$. Finally, a bound to $\|G_y\|^2$ follows from

$$\|R'\|^2_{L^2(0,d)} \;=\; \frac{\pi}{4a} + \left(\frac{2}{d} - \frac{\pi}{4a}\right) e^{-\pi d/2a} \;<\; \frac{\pi}{4a}$$

for $a < \pi d/8$, which means that $\|G_y\|^2 < \eta^2\pi/4$. Putting these estimates together, using $\|F_x\|^2 = \alpha^2\kappa$, and neglecting the negative term $-\left(\frac{\pi}{d}\right)^2 \|G\|^2$, we arrive at the inequality

$$L(\psi) \;<\; \alpha^2\kappa - \frac{8\sqrt{2}\,\alpha a}{d^{3/2}}\,\eta + \frac{\pi}{4}\,(2+\varepsilon_1)\eta^2\,,$$

where the sum of the last two terms at the *rhs* is minimized by $-\frac{2^7\alpha^2 a^2}{\pi d^3(2+\varepsilon_1)}$. It remains to estimate $\|\psi\|^2$ from below. The tail contribution is $\|\psi\|^2_{|x|\ge a} = \alpha^2/\kappa$, while the window part expresses as

$$\|\psi\|^2_{|x|\le a} \;\le\; 2\|F\|^2_{|x|\le a} + 2\|G\|^2_{|x|\le a} \;=\; 4a\alpha^2 + 2a\eta^2\|R\|^2_{L^2(0,d)} \;<\; Ca$$

for some $C > 0$; this means that $\|\psi\|^2 > \alpha^2(1-\varepsilon_2)\kappa^{-1}$ holds for any $\varepsilon_2 > 0$ and all a small enough. Hence

$$\frac{L(\psi)}{\|\psi\|^2} < (1-\varepsilon_2)^{-1}\left(\kappa^2 - \frac{2^7 a^2 \kappa}{\pi d^3(1+\varepsilon_1)}\right) ;$$

taking the minimum over κ we find

$$\frac{L(\psi)}{\|\psi\|^2} < (1-\varepsilon_2)^{-1}\frac{2^{12}a^4}{\pi^2 d^6(1+\varepsilon_1)^2}, \tag{3.5}$$

which completes the proof of the first inequality of (2.1) in the symmetric case, $d_1 = d_2$.

Let us pass to the nonsymmetric case and suppose for definiteness that $d = d_1 > d_2$; the bottom of the essential spectrum is then determined by the upper part of Σ. We choose there the same trial function as above, *i.e.*, $\psi = F+G$ is for $y \ge 0$ given by (3.1) and (3.2). Let further R_2 be defined by (3.3) with d, y replaced by d_2 and $-y$, respectively. In the lower part of the strip, $I\!R\times[-d_2,0]$, we put $\psi = G$ where G is given by (3.2) with R replaced by R_2. The trial function should be smoothed in the window by requiring the continuity, $G^\varepsilon(x,0+) = G^\varepsilon(x,0-)$, and

$$G^\varepsilon_y(x,0+) = -\frac{\sqrt{2}\,\alpha\pi}{d^{3/2}}, \qquad G^\varepsilon_y(x,0-) = 0\,.$$

Then it belongs to $Q(H)$; in the same way as above it is sufficient to compute the functional for the nonsmoothed ψ. The value of $L(\psi)$ can be estimated by

$$L(\psi) < \alpha^2\kappa - \frac{8\sqrt{2}\,\alpha a}{d^{3/2}}\eta + \frac{\pi}{2}(2+\varepsilon_1)\eta^2,$$

and since the contribution to $\|\psi\|^2$ from the window part is again $\mathcal{O}(a)$, the argument used in the symmetric case may be repeated. ∎

4 Two lemmas

To prove the other part of Theorem 2.2 we need a few variational results for real–valued functions. Let us first mention two elementary inequalities obtained directly by solving the appropriate Euler equations. Let $\phi \in C^2(I\!R_+)$ with $\phi(0) = \alpha$; then

$$\int_0^\infty \left(\phi'(t)^2 + m^2\phi^2(t)\right)(t)\,dt \ge m\alpha^2 \tag{4.1}$$

holds for a fixed $m \ge 0$. Similarly, if $\phi \in C^2[-b,b]$ with $\phi(\pm b) = 0$, then

$$\int_{-b}^b \phi'(t)^2 dt \ge \left(\frac{\pi}{2b}\right)^2 \int_{-b}^b \phi(t)^2 dt\,. \tag{4.2}$$

The following results are a little more involved:

Lemma 4.1 *Let $\phi \in C^2[0,d]$ be a function with $\phi(d)=0$; then there are positive $\varepsilon_1, \varepsilon_2$ such that $\left|\int_0^d \phi(t)\chi_1(t)\,dt\right| < \varepsilon_1\|\phi\|$ implies*

$$\int_{-d}^{d} \phi'(t)^2 dt \,>\, (1+\varepsilon_2)\left(\frac{\pi}{d}\right)^2 \|\phi\|^2 . \tag{4.3}$$

Proof. Let $\{g_n\}$ be the "Dirichlet" trigonometric basis in $L^2(-d,d)$; in particular, $2^{1/2}g_2$ is the odd extension of χ_1. We denote by Φ the even extension of ϕ to $[-d,d]$; without loss of generality we may suppose that it has a unit norm. Since Φ is even by assumption, we write it as $\Phi = \gamma_1 g_1 + h$ with $h \in \{g_1, g_2\}^{\perp}$ which implies

$$\|\Phi'\|^2 = \gamma_1^2\left(\frac{\pi}{2d}\right)^2 + \|h'\|^2 , \qquad \|h'\|^2 \ge \left(\frac{3\pi}{2d}\right)^2 \|h\|^2 . \tag{4.4}$$

In a similar way we have $\xi = \xi_1 g_1 + \tilde\xi$ for the even function $\xi := |g_2|$. We find easily $\xi_1 = 8/3\pi$, so $\|\tilde\xi\| = \sqrt{1-\xi_1^2} \approx 0.529$.

If $|(\xi,\Phi)| < 2^{3/2}\varepsilon_1$, the identities $\xi_1\gamma_1 = (\xi,\Phi) - (\tilde\xi, h)$ and $\|h\|^2 = 1-\gamma_1^2$ yield

$$\frac{8}{3\pi}\,|\gamma_1| \,\le\, \varepsilon_1\sqrt{2} + \sqrt{1-\gamma_1^2}\,\sqrt{1-\left(\frac{8}{3\pi}\right)^2} .$$

This requires

$$|\gamma_1| \,\le\, \frac{8\sqrt{2}}{3\pi}\,\varepsilon_1 \,+\, \sqrt{(1-2\varepsilon_1^2)\left(1-\left(\frac{8}{3\pi}\right)^2\right)} \; ;$$

hence choosing ε_1 small enough we achieve $|\gamma_1| > \frac{1}{2}$. Consequently, $\|\Phi'\|^2 > \frac{7\pi^2}{4d^2}$ holds in view of (4.4). ∎

Lemma 4.2 *Let $\phi \in C^2[0,d]$ with $\phi(0)=\beta$ and $\phi(d)=0$. If $(\phi,\chi_1)=0$, then for every $m>0$ there is $c_0>0$ such that*

$$\int_0^d \phi'(t)^2 dt \,+\, \left(\frac{m}{a}\right)^2 \int_0^a \phi(t)^2 dt \,-\, \left(\frac{\pi}{d}\right)^2 \int_0^d \phi(t)^2 dt \,\ge\, \frac{c_0\beta^2}{a} \tag{4.5}$$

holds for all a small enough.

Proof. We denote the *lhs* of (4.5) by $M(\phi)$ and use subscripts to mark a contribution to a norm from a particular interval. Furthermore, we introduce

$$\tilde\phi(x) \,:=\, \begin{cases} \phi(a) & \dots \quad 0 \le x \le a \\ \phi(x) & \dots \quad a \le x \le d \end{cases} \tag{4.6}$$

Notice that $\|\chi_1\|_{t\le a} \to 0$ as $a \to 0$, so there is $a_0 > 0$ such that $2\|\chi_1\|_{t\le a} < \varepsilon_1$ holds for $a < a_0$, where ε_1 is the positive number from the previous lemma; we shall restrict ourselves in the following to

$$a \,<\, \min\left\{ a_0,\, \frac{md}{\pi\sqrt{3}} \right\} . \tag{4.7}$$

Suppose first that

$$\|\phi\|_{t\le a}^2 > \|\tilde\phi\|^2 \tag{4.8}$$

holds for some ϕ. Since the *rhs* is not smaller than $\|\phi\|_{t\ge a}^2$, we have in view of (4.7)

$$\max\left\{ \left(\frac{\pi}{d}\right)^2 \|\phi\|_{t\le a}^2,\, \left(\frac{\pi}{d}\right)^2 \|\phi\|_{t\ge a}^2 \right\} < \frac{m^2}{3a^2}\, \|\phi\|_{t\le a}^2\,,$$

so neglecting the non–negative term $\|\phi'\|_{t\ge a}^2$, we arrive at the estimate

$$M(\phi) > \|\phi'\|_{t\le a}^2 + \frac{m^2}{3a^2}\, \|\phi\|_{t\le a}^2 \ge \frac{\beta^2 m}{a\sqrt{3}} \tanh \frac{m}{\sqrt{3}}\,; \tag{4.9}$$

the last inequality follows from the fact that the estimating functional is for a fixed $\alpha := \phi(a)$ minimized by $\phi(t) = \frac{\beta}{\sinh\mu}\, (\alpha \sinh\mu t + \sinh\mu(a-t))$, where $\mu := \frac{m}{\sqrt{3}}$, and taking the minimum over α. Consider on the contrary those ϕ for which (4.8) is violated, *i.e.*,

$$\|\phi\|_{t\le a}^2 \le \|\tilde\phi\|^2\,. \tag{4.10}$$

Since ϕ is by assumption orthogonal to χ_1, we have

$$\int_0^d \tilde\phi(t)\chi_1(t)\, dt = \int_0^a \tilde\phi(t)\chi_1(t)\, dt - \int_0^a \phi(t)\chi_1(t)\, dt\,,$$

so

$$\left| \int_0^d \tilde\phi(t)\chi_1(t)\, dt \right| \le \left(\|\tilde\phi\|_{t\le a} + \|\phi\|_{t\le a} \right) \|\chi_1\|_{t\le a} \le 2\|\chi_1\|_{t\le a} \|\tilde\phi\| < \varepsilon_1 \|\tilde\phi\|\,;$$

applying Lemma 4.1 to $\tilde\phi$ we obtain

$$\int_a^d \phi'(t)^2 dt - \left(\frac{\pi}{d}\right)^2 \int_a^d \phi(t)^2 dt \ge \int_0^d \tilde\phi'(t)^2 dt - \left(\frac{\pi}{d}\right)^2 \int_a^d \tilde\phi(t)^2 dt > \varepsilon_2 \left(\frac{\pi}{d}\right)^2 \|\tilde\phi\|^2$$

for some $\varepsilon_2 > 0$. Neglecting this non–negative term, we get

$$M(\phi) > \|\phi'\|_{t\le a}^2 + \frac{m^2}{a^2}\, \|\phi\|_{t\le a}^2 - \left(\frac{\pi}{d}\right)^2 \|\phi\|_{t\le a}^2\,; \tag{4.11}$$

then it is sufficient to employ (4.7) and estimate the *rhs* in the same way as in (4.9) to arrive at the desired conclusion. ∎

5 A lower bound

This is the most difficult part of the proof. However, we may restrict ourselves to the symmetric case only because inserting an additional Neumann boundary into the window we get a lower bound to $H(d_1, d_2; 2a)$; hence it is sufficient to treat the spectrum of $H \equiv H(d; 2a)$.

We have to estimate $L(\psi) := (H\psi,\psi) - \left(\frac{\pi}{d}\right)^2 \|\psi\|^2$ over $\|\psi\|^2$ for all ψ of a core of H, say, all C^2–smooth $\psi \in L^2(\Sigma_+)$ satisfying the boundary conditions. We shall employ for such functions and $|x| \geq a$ the following uniformly convergent Fourier expansion

$$\psi(x,y) \;=\; \sum_{n=1}^{\infty} c_n(x)\chi_n(y)\,, \tag{5.1}$$

where the coefficients $c_n(x) = (\psi(x,\cdot),\chi_n)$ are again smooth. Some natural restrictions may be adopted:

(i) only real–valued ψ should be taken into account: since H commutes with complex conjugation we may consider $L^2(\Sigma_+)$ as a real Hilbert space in which H is "doubled",

(ii) we may consider x–even ψ only, because due to mirror symmetry we have $H = H_{even} \oplus H_{odd}$, where the two parts are unitarily equivalent to the half-strip Laplacian with the Neumann and Dirichlet condition, respectively, at the transverse cut. Hence $H_{even} \leq H_{odd}$, and it is sufficient to estimate the even part only.

Next we have to introduce some more notation. We put $c_1 = f_1 + \hat f_1$, where

$$\hat f_1 \;:=\; \left\{ \begin{array}{lll} 0 & \dots & |x| \geq 2a \\ c_1(x) - \alpha & \dots & |x| \geq 2a \end{array} \right. \tag{5.2}$$

with $\alpha := c_1(2a)$, so $\hat f_1(\pm 2a) = 0$, and furthermore

$$\psi(x,y) \;=\; F(x,y) + G(x,y)\,, \qquad F(x,y) \;:=\; f_1(x)\chi_1(y)\,. \tag{5.3}$$

Using this decomposition we derive in the same way as in Section 3 an expression for the functional to be estimated,

$$L(\psi) \;=\; \|\psi_x\|^2 + \|G_y\|^2 - \left(\frac{\pi}{d}\right)^2 \|G\|^2 - 2\alpha\,\frac{\pi}{d}\sqrt{\frac{2}{d}}\int_{-a}^{a} G(x,0)\,dx\,. \tag{5.4}$$

Let us begin with the contribution from the outer region. We split a half of the first term and consider the following expression:

$$\begin{aligned} &\frac{1}{2}\,\|\psi_x\|^2_{|x|\geq a} + \|G_y\|^2_{|x|\geq a} - \left(\frac{\pi}{d}\right)^2 \|G\|^2_{|x|\geq a} \\ &\quad = \sum_{n=1}^{\infty}\int_a^{\infty} c_n'(x)^2\,dx \;+\; 2\sum_{n=1}^{\infty}\left(\frac{\pi}{d}\right)^2 \left(n^2-1\right)\int_a^{\infty} c_n(x)^2\,dx\,. \end{aligned}$$

Since

$$\int_a^{\infty}\left[\frac{1}{2}\,c_n'(x)^2\,dx + \left(\frac{\pi}{d}\sqrt{n^2-1}\right)^2 c_n(x)^2\right]dx \;>\; \frac{\pi n}{2d}\,c_n(a)^2$$

by (4.1) for $n \geq 2$, and the non–negative term $\int_a^\infty c_1'(x)^2\, dx$ may be neglected, we have

$$\frac{1}{2}\, \|\psi_x\|^2_{|x|\geq a} + \|G_y\|^2_{|x|\geq a} - \left(\frac{\pi}{d}\right)^2 \|G\|^2_{|x|\geq a} \;>\; \frac{\pi}{d} \sum_{n=2}^{\infty} n c_n(a)^2\,,$$

and therefore

$$\begin{aligned} L(\psi) \;>\; & \frac{1}{2}\, \|\psi_x\|^2_{|x|\geq a} + \|G_x\|^2_{|x|\leq a} + \|G_y\|^2_{|x|\leq a} - \left(\frac{\pi}{d}\right)^2 \|G\|^2_{|x|\leq a} \\ & + \; \frac{\pi}{d} \sum_{n=2}^{\infty} n c_n(a)^2 - \; 2\alpha\, \frac{\pi}{d} \sqrt{\frac{2}{d}} \int_{-a}^{a} G(x,0)\, dx\,, \end{aligned} \tag{5.5}$$

where we have also employed the fact that $\psi_x = G_x$ for $|x| \leq 2a$.

Our next goal is to estimate the sum of the first two terms in (5.5) by estimating $\|G_x\|^2_{|x|\leq 2a}$. If a function $\tilde{G} : \Sigma_+ \to C^2(\Sigma_+)$ vanishes at $x = \pm 2a$, the inequality (4.2) implies

$$\|\tilde{G}_x\|^2_{|x|\leq 2a} \;\geq\; \left(\frac{\pi}{4a}\right)^2 \|\tilde{G}\|^2_{|x|\leq 2a}\,. \tag{5.6}$$

Unfortunately, G does not satisfy this requirement, which forces us to split it into several components and to estimate them separately. First we single out the projection of G onto the first transverse mode,

$$G(x,y) \;=\; G_1(x,y) + G_2(x,y)\,, \qquad G_1(x,y) \;=\; \hat{f}_1(x)\chi_1(y)\,. \tag{5.7}$$

Since $\hat{f}_1(\pm 2a) = 0$ by definition, (5.6) may be applied to G_1. In combination with the inequality

$$\frac{1}{2}\, \|\psi_x\|^2_{a\leq|x|\leq 2a} + \; \|G_x\|^2_{|x|\leq a} \;\geq\; \frac{1}{2}\, \|G_x\|^2_{|x|\leq 2a} \;=\; \frac{1}{2}\, \|G_{1,x}\|^2_{|x|\leq 2a} + \; \frac{1}{2}\, \|G_{2,x}\|^2_{|x|\leq 2a}\,,$$

where the subscript in the last norm may be dropped because $G_1(x,y) = 0$ for $|x| \geq 2a$, we get

$$\begin{aligned} L(\psi) \;>\; & \frac{1}{2}\, \|\psi_x\|^2_{|x|\geq 2a} + \; \frac{1}{2}\, \|G_{2,x}\|^2_{|x|\leq 2a} + \|G_y\|^2_{|x|\leq a} - \left(\frac{\pi}{d}\right)^2 \|G\|^2_{|x|\leq a} \\ & + \; \frac{\pi}{d} \sum_{n=2}^{\infty} n c_n(a)^2 - \; 2\alpha\, \frac{\pi}{d} \sqrt{\frac{2}{d}} \int_{-a}^{a} G(x,0)\, dx \; + \; \frac{\pi^2}{32a^2}\, \|G_1\|^2\,. \end{aligned} \tag{5.8}$$

The function G_2 has again to be splitted; we rewrite it as

$$G_2(x,y) \;=\; \hat{G}(x,y) + \Gamma(x,y)\,, \qquad \Gamma(x,y) \;:=\; \sum_{n=2}^{\infty} c_n(2a)\chi_n(y)\,, \tag{5.9}$$

for $|x| \leq 2a$; the second part is independent of x while the first one vanishes at the border, $|x| = 2a$, so $G_{2,x} = \hat{G}_x$ may be estimated by means of (5.6) and the Schwarz inequality as

$$\|G_{2,x}\|^2_{|x|\leq 2a} \geq \left(\frac{\pi}{4a}\right)^2 \|\hat{G}\|^2_{|x|\leq 2a} \;\geq\; \frac{1}{2} \left(\frac{\pi}{4a}\right)^2 \|G_2\|^2_{|x|\leq 2a} - \left(\frac{\pi}{4a}\right)^2 \|\Gamma\|^2_{|x|\leq 2a}. \tag{5.10}$$

However, it is difficult to find a suitable bound for the last negative term. Instead of attempting it we restrict ourselves to the vicinity of the window: we introduce $\Omega_a := [-2a, 2a] \times [0, a]$ and replace (5.10) by

$$\|G_{2,x}\|^2_{|x|\le 2a} \ge \left(\frac{\pi}{4a}\right)^2 \|\hat{G}\|^2_{|x|\le 2a} \ge \left(\frac{\pi}{4a}\right)^2 \|\hat{G}\|^2_{\Omega_a} \ge \frac{1}{2}\left(\frac{\pi}{4a}\right)^2 \|G_2\|^2_{\Omega_a} - \left(\frac{\pi}{4a}\right)^2 \|\Gamma\|^2_{\Omega_a}. \tag{5.11}$$

We have still to find an upper bound to $\|\Gamma\|^2_{\Omega_a}$. To this end we notice that, in addition to *(i)*, *(ii)*, we may restrict our attention to those ψ for which

$$|c_n(x)| \le |c_n^{ex}(x)|, \qquad c_n^{ex}(x) := c_n(a)\, e^{-(\pi/d)\sqrt{n^2-1}(x-a)}, \tag{5.12}$$

holds for $|x| \ge a$ and $n \ge 2$. Indeed, let us split ψ for $|x| \ge a$ into a contribution from the n–th transverse mode, $n \ge 2$, and the orthogonal complement introducing

$$\tilde{\psi}(x,y) := \left\{ \begin{array}{lll} \psi(x,y) & \dots & |x| < a \\ \psi(x,y) - c_n(x)\chi_n(y) & \dots & |x| \ge a \end{array} \right.$$

The basic expression to be estimated can be then written as

$$\frac{L(\psi)}{\|\psi\|^2} = \frac{\left(H\tilde{\psi}, \tilde{\psi}\right) - \left(\frac{\pi}{d}\right)^2 \|\tilde{\psi}\|^2 + 2\int_a^\infty \left[c_n'(x)^2\, dx + \left(\frac{\pi}{d}\sqrt{n^2-1}\right)^2 c_n(x)^2 \right] dx}{\|\tilde{\psi}\|^2 + 2\int_a^\infty c_n(x)^2 dx}.$$

Without loss of generality we may assume only those ψ for which the numerator is negative. The part of its last term corresponding to the interval $[a, \infty)$ is by (4.1) minimized by the exponential function $|c_n^{ex}|$ of (5.12); hence replacing $c_n(x)^2$ by $\min\{c_n(x)^2, c_n^{ex}(x)^2\}$ we can only get a larger negative number. At the same time, the positive denominator can be only diminished, which justifies the claim made above.

We are interested in the norm of Γ restricted to Ω_a, hence we cannot use the Parseval relation because in general the restrictions of χ_n to $[0, a]$ are not orthogonal. We divide therefore the series into two pieces referring to small and large values, respectively, relative to a^{-1}. In the first part we employ the smallness of the χ_n norm restricted to $[0, a]$, while the other part will be estimated by means of the subexponential decay (5.12). In this way, we may write

$$\begin{aligned}
\|\Gamma\|^2_{\Omega_a} &= \int_{-2a}^{2a} dx \int_0^a dy \left(\sum_{n=2}^{\infty} c_n(2a)\chi_n(y) \right)^2 \\
&\le 8a \int_0^a \left(\sum_{n=2}^{[a^{-1}]+1} c_n(2a)\chi_n(y) \right)^2 dy + 8a \int_0^a \left(\sum_{2\le n=[a^{-1}]+2}^{\infty} c_n(2a)\chi_n(y) \right)^2 dy \\
&\le 8a \left(\sum_{n=2}^{[a^{-1}]+1} n^{-1} c_n(a)^2 \int_0^a \chi_n(y)^2 dy \right) \left(\sum_{n=2}^{[a^{-1}]+1} n \right) \\
&+ 8a \left(\sum_{2\le n=[a^{-1}]+2}^{\infty} n c_n(a)^2 \int_0^a \chi_n(y)^2 dy \right) \left(\sum_{2\le n=[a^{-1}]+2}^{\infty} n^{-1} e^{-(2\pi a/d)\sqrt{n^2-1}} \right),
\end{aligned}$$

where $[\cdot]$ denotes the entire part; in the first term on the *rhs* we have used the rough bound $c_n(2a) < c_n(a)$. The transverse–mode integral equals

$$\int_0^a \chi_n(y)^2 dy \,=\, \frac{a}{d}\left[1-\left(\frac{d}{2\pi na}\right)\sin\left(\frac{2\pi na}{d}\right)\right] \,\le\, \frac{a}{d}\,\min\left\{\frac{1}{6}\left(\frac{2\pi na}{d}\right)^2,\, 2\right\}\,;$$

being small for small a as indicated. We arrive thus at the inequality

$$\|\Gamma\|^2_{\Omega_a} \,\le\, \frac{16a^2}{d}\left\{\frac{2\pi^2}{3d^2} + \sum_{n=[a^{-1}]+1}^{\infty} n^{-1}e^{-2\pi an/d}\right\}\sum_{n=2}^{\infty} nc_n(a)^2\,, \tag{5.13}$$

where we have employed the estimates $\sum_{n=2}^{[a^{-1}]+1} n \,\le\, 2a^{-1}$ and $\sqrt{n^2-1} \,<\, n-1$. The sum in the curly bracket at the *rhs* of (5.13) has a uniform upper bound with respect to a being a Darboux sum of the integral

$$\int_1^\infty \frac{e^{-2\pi x/d}}{x}\,dx \,=\, -\,\mathrm{Ei}\left(-\,\frac{2\pi}{d}\right)\,,$$

where Ei is the exponential integral function. Hence there is a positive C such that

$$\|\Gamma\|^2_{\Omega_a} \,\le\, Ca^2\sum_{n=2}^{\infty} nc_n(a)^2\,. \tag{5.14}$$

By (5.11) we have

$$\frac{1}{2}\,\|G_{2,x}\|^2_{|x|\le 2a} + \frac{\pi}{d}\sum_{n=2}^{\infty} nc_n(a)^2 \ge \frac{\delta}{4}\left(\frac{\pi}{4a}\right)^2\|G_2\|^2_{\Omega_a} - \frac{\delta}{2}\,\|\Gamma\|^2_{\Omega_a} + \frac{\pi}{d}\sum_{n=2}^{\infty} nc_n(a)^2$$

for any $\delta\in(0,1]$; the estimate (5.14) shows that choosing δ small enough one can achieve that the sum of the last two terms is non–negative. Putting $m := \frac{\pi}{8}\sqrt{\delta}$, we arrive at the bound

$$\begin{aligned} L(\psi) \,&>\, \frac{1}{2}\,\|\psi_x\|^2_{|x|\ge 2a} + \|G_y\|^2_{|x|\le a} - \left(\frac{\pi}{d}\right)^2\|G\|^2_{|x|\le a} + \frac{\pi^2}{32a^2}\,\|G_1\|^2 \\ &-\, 2\alpha\,\frac{\pi}{d}\sqrt{\frac{2}{d}}\int_{-a}^{a} G(x,0)\,dx \,+\, \frac{m^2}{a^2}\,\|G_2\|^2_{\Omega_a}\,. \end{aligned} \tag{5.15}$$

In the next step we express the term containing G_y using the decomposition (5.7), a simple integration by parts, the relation $G_2(x,0) = G(x,0)$, and the fact that $G_2(x,\cdot)$ is orthogonal to $\chi_1'' = -(\pi/d)^2\chi_1$. This yields

$$\|G_y\|^2_{|x|\le a} = \|G_{1,y}\|^2_{|x|\le a} + \|G_{2,y}\|^2_{|x|\le a} - 2\,\frac{\pi}{d}\sqrt{\frac{2}{d}}\int_{-a}^{a}\hat f_1(x)G(x,0)\,dx\,,$$

where the last term does not exceed $(\pi/d^2)\left(2\|G_1\|^2_{|x|\le a} + d\|G(\cdot,0)\|^2_{|x|\le a}\right)$ by the Schwarz inequality. We substitute to (5.15) from here keeping in mind the identity $\|G\|^2_{|x|\le a} = \|G_1\|^2_{|x|\le a} + \|G_2\|^2_{|x|\le a}$, and neglect the term $\|G_{1,y}\|^2_{|x|\le a}$ as well as

$$\frac{\pi^2}{32a^2}\,\|G_1\|^2 - \frac{\pi(\pi+2)}{d^2}\,\|G_{1,y}\|^2_{|x|\le a}$$

which is positive for a small enough, obtaining

$$
\begin{aligned}
L(\psi) \;>\; & \frac{1}{2}\,\|\psi_x\|^2_{|x|\geq 2a} + \|G_{2,y}\|^2_{|x|\leq a} + \frac{m^2}{a^2}\,\|G_2\|^2_{\Omega_a} - \left(\frac{\pi}{d}\right)^2 \|G_2\|^2_{|x|\leq a} \\
& - \frac{\pi}{d}\,\|G_2(\cdot,0)\|^2_{|x|\leq a} - 2\alpha\,\frac{\pi}{d}\sqrt{\frac{2}{d}}\int_{-a}^{a} G_2(x,0)\,dx\,.
\end{aligned}
\tag{5.16}
$$

Furthermore, the function $G_2(x,\cdot)$ satisfies for a fixed $x\in[-a,a]$ the assumptions of Lemma 4.2, so the sum of the second, third, and fourth term on the *rhs* is below bounded by $(c_0/a)\,\|G_2(\cdot,0)\|^2_{|x|\leq a}$. Since $(c_0/2a)-(\pi/d)>0$ for small a, we have

$$
L(\psi) \;>\; \frac{1}{2}\,\|\psi_x\|^2_{|x|\geq 2a} + \frac{c_0}{2a}\,\|G_2(\cdot,0)\|^2_{|x|\leq a} - 2\alpha\,\frac{\pi}{d}\sqrt{\frac{2}{d}}\,\|G_2(\cdot,0)\|_{|x|\leq a}\sqrt{2a}\,,
$$

where we have employed the Schwarz inequality again; taking the minimum over $\|G_2(\cdot,0)\|_{|x|\leq a}$, we arrive finally at the estimate

$$
L(\psi) \;>\; \frac{1}{2}\,\|\psi_x\|^2_{|x|\geq 2a} - \frac{8\pi^2\alpha^2}{c_0 d^3}\,. \tag{5.17}
$$

The rest of the argument is simple. We have $\|\psi\|^2 \geq \|\psi\|^2_{|x|\geq 2a} \geq 2\int_{2a}^{\infty} c_1(x)^2dx$, and a similar bound is valid for the first term on the *rhs* of (5.17), so

$$
\frac{L(\psi)}{\|\psi\|^2} \;>\; \frac{\int_{2a}^{\infty} c_1'(x)^2dx \;-\; \frac{8\pi^2\alpha^2}{c_0d^3}}{2\int_{2a}^{\infty} c_1(x)^2dx}\,.
$$

The extremal of this functional over functions with a fixed value at $x=2a$ is $c_1(2a)\,e^{-\kappa(x-2a)}$ which yields the value $(\kappa^2/2)-(8\pi^2/c_0d^3)\kappa a^2$. It is now sufficient to take the minimum over κ to get the inequality

$$
\frac{L(\psi)}{\|\psi\|^2} \;>\; -\,2\left(\frac{4\pi^2}{c_0d^3}\right)^2 a^4\,, \tag{5.18}
$$

which completes the proof of Theorem 2.2. ∎

Remark 5.1 Some of the estimates we used are certainly crude, however, pushing them to an optimum is not sufficient to squeeze the bound (2.1) enough to get the actual asymptotic behavior. This question remains open; the same is true for the window–width threshold behavior of higher eigenvalues [ESTV].

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