A lower bound to the spectral threshold in curved quantum layers

Pedro Freitas and David Krejčířík

Abstract. We derive a lower bound to the spectral threshold of the Dirichlet Laplacian in tubular neighbourhoods of constant radius about complete surfaces. This lower bound is given by the lowest eigenvalue of a one-dimensional operator depending on the radius and principal curvatures of the reference surface. Moreover, we show that it is optimal if the reference surface is non-negatively curved.

1. Introduction

In this paper we obtain a lower bound to the lowest energy of a quantum particle confined to the space delimited by two parallel surfaces. We assume that these surfaces represent a perfect hard-wall boundary, in the sense that the particle wave-function vanishes there, and concentrate in the case where they are unbounded. In agreement with the paper [6] where these structures were introduced, we shall use the term quantum layers for such systems.

This rather simple model is known to be remarkably successful in describing various aspects of electronic transport in quantum heterostructures (we refer to the monograph [20] for the physical background). One of the main questions arising within this scope is whether or not there are geometrically induced bound states. Indeed, some of the most important theoretical results in the field are a number of theorems guaranteeing the existence of such solutions under rather simple and general physical conditions [6, 9, 15, 17, 19, 21] (see also [9, 13, 12, 14, 11, 5, 13, 15] for other mathematical studies of quantum layers).

The main contribution of the present paper is to provide a lower bound to the ground-state energy of the bound states. However, our results are more general in the sense that this lower bound also applies to situations where the lowest energy in the spectrum does not correspond to a bound state, but rather to a scattering state; this happens, e.g., if the layer is periodically curved.

To obtain this lower bound, we follow an idea similar to that used by Pavel Exner and the present authors in [8] to derive a lower bound to the spectral threshold in quantum tubes, i.e. in the case of the configuration space being a $d$-dimensional tube about an infinite curve, with $d \geq 2$. More precisely, there it was shown that the lower bound is given by the lowest Dirichlet eigenvalue in a torus determined by the geometry of the tube. This lower bound is optimal in the sense that it is achieved by a tube (about a curve of constant curvature). However,
the geometry of quantum layers is more complicated and we shall see that the optimality is one of the main features in which the present situation differs from that of quantum tubes.

In view of the above physical model, the Hamiltonian of a quantum layer can be identified with the Dirichlet Laplacian in a tubular neighbourhood of constant radius about a complete non-compact surface $\Sigma \subset \mathbb{R}^3$. In this paper, we proceed in a greater generality by considering compact surfaces, too. More precisely, we assume only that

$$\Sigma$$ is a connected complete orientable surface of class $C^2$ embedded in $\mathbb{R}^3$ with bounded principal curvatures $k_1$ and $k_2$.\(^{(1)}\)

Then, given a positive number $a$ satisfying

$$a \max\{\|k_1\|_\infty, \|k_2\|_\infty\} < 1,$$

we introduce the tubular neighbourhood

$$\Omega := \{x \in \mathbb{R}^3 \mid \text{dist}(x, \Sigma) < a\}$$

and denote by $-\Delta^\Omega_D$ the Dirichlet Laplacian in $L^2(\Omega)$. In addition to (2), we also assume that $\Omega$ “does not overlap itself” (cf. (8) below).

If $\Sigma$ is compact, then $\Omega$ is bounded and a lower bound to the spectral threshold of the Laplacian follows by means of the Faber-Krahn inequality; i.e., $\inf \sigma(-\Delta^\Omega_D)$ is bounded from below by the lowest Dirichlet eigenvalue of the ball of volume $|\Omega|$ in this case. However, we are mainly interested in the unbounded case, where similar arguments based on the Faber-Krahn inequality may, at best, just provide a trivial bound and the location of $\inf \sigma(-\Delta^\Omega_D)$ becomes difficult, since we are actually dealing with a class of quasi-cylindrical domains (cf. [10, §49] or [7, Sec. X.6.1]).

In this note we derive the following universal lower bound:

**Theorem 1.** Let $\Omega$ be as above. One has

$$\inf \sigma(-\Delta^\Omega_D) \geq \min \{\lambda_1(k_1^+, k_2^-), \lambda_1(k_1^-, k_2^+)\},$$

where $k_i^\pm := \pm \sup(\pm k_i)$, $i \in \{1, 2\}$, and

$$\lambda_1(\kappa_1, \kappa_2) := \inf_{\psi \in W_0^{1,2}(((-a,a)) \setminus \{0\})} \frac{\int_{-a}^a |\psi'(u)|^2 \left(1 - \kappa_1 u\right) \left(1 - \kappa_2 u\right) \, du}{\int_{-a}^a |\psi(u)|^2 \left(1 - \kappa_1 u\right) \left(1 - \kappa_2 u\right) \, du}$$

for constants $\kappa_1, \kappa_2 \in [-1/a, 1/a]$.

In view of Theorem 1, the spectral threshold of the Dirichlet Laplacian in the three-dimensional tubular manifold $\Omega$ can be estimated from below by means of the one-dimensional spectral problem associated with (5). It is easy to verify that $\lambda_1(k_1, k_2)$ with constant $k_1$ and $k_2$ gives the spectral threshold of the Dirichlet
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Laplacian in the layer about the plane if \( k_1 = k_2 = 0 \), a sphere if \( k_1 = k_2 > 0 \) or a cylinder if \( k_1 > 0 \) and \( k_2 = 0 \). That is, Theorem \( 1 \) is optimal for the class of layers built about surfaces with non-negative Gauss curvature \( k_1 k_2 \). On the other hand, we are not aware of a geometric meaning of (5) if the Gauss curvature \( k_1 k_2 \) is negative and the surface is complete. In fact, since no such surface exists which satisfies hypothesis (1) and whose Gauss curvature is identically equal to a negative constant, a better lower bound than (5) is expected to hold for layers about surfaces with sign-changing or non-positive Gauss curvature.

In any case, while the right hand side of (4) diminishes as the Gauss curvature of \( \Sigma \) becomes more negative, it is uniformly bounded away from zero for layers about surfaces whose Gauss curvature is non-negative:

**Proposition 1.** Let \( \kappa_1, \kappa_2 \in (-1/a, 1/a) \) be such that \( \kappa_1 \kappa_2 \geq 0 \). Then

\[
\lambda_1(\kappa_1, \kappa_2) \geq j_{0,1}^2/(2a)^2,
\]

where \( j_{0,1} \approx 2.40 \) denotes the first zero of the Bessel function \( J_0 \).

The bound of Proposition \( 1 \) is reminiscent of the uniform lower bound obtained in \( 8 \) for strips, i.e. a two-dimensional analogy of quantum layers, by applying the Faber-Krahn inequality to a sequence of Dirichlet annuli converging to a Dirichlet disk.

If \( \kappa_1 \kappa_2 < 0 \), it actually turns out that it is impossible to obtain a lower bound to \( \lambda_1(\kappa_1, \kappa_2) \) for all \( \kappa_1, \kappa_2 \in (-1/a, 1/a) \) that would not depend on \( \kappa_1 \) and \( \kappa_2 \), as the following result shows:

**Proposition 2.** We have

\[
\lambda_1(-1/a, 1/a) = 0.
\]

The rest of this paper consists of one section where we provide the proofs of Theorem \( \ref{thm:1} \) and Propositions \( \ref{prop:1} \) and \( \ref{prop:2} \).

2. The proofs

The central step in the proof of Theorem \( \ref{thm:1} \) is based on an idea adopted from \( 8 \). Roughly speaking, expressing the Laplacian \(-\Delta_D^\Sigma \) in the natural coordinates parameterising the layer \( 3 \) by means of “longitudinal” coordinates of the reference surface \( \Sigma \) and a “transverse” coordinate of the normal bundle of \( \Sigma \), we neglect the contribution of the former and the latter leads to a “variable” lower bound of the type \( 5 \). The constant lower bound given by the right hand side of (4) and the uniform lower bound of Proposition \( \ref{prop:1} \) then follow from an analysis of the one-dimensional spectral problem associated with (5).

We need to start with a detailed geometry of curved layers adopted from \( 3 \). Let \( g \) be the Riemannian metric of \( \Sigma \) induced by the embedding. The orientation of \( \Sigma \) is specified by a globally defined unit normal vector field \( n : \Sigma \to S^2 \). For any point \( x \in \Sigma \), we introduce the Weingarten map

\[
L_x : T_x \Sigma \to T_x \Sigma : \{ \xi \mapsto -dn_x(\xi) \}.
\]
The principal curvatures $k_1$ and $k_2$ at $x$ are defined as eigenvalues of $L_2$ with respect to $g(x)$. Although these curvatures are a priori defined only locally on $\Sigma$, the Gauss curvature $K := k_1 k_2$ and the mean curvature $M := \frac{1}{2}(k_1 + k_2)$ are globally defined continuous functions on $\Sigma$.

Let us introduce the mapping
\[
\mathcal{L} : \Sigma \times (-a, a) \to \mathbb{R}^3 : \{(x, u) \mapsto x + n(x) u\}.
\]
Assuming (2) and that $\mathcal{L}$ is injective, this mapping induces a diffeomorphism and the image $\mathcal{L}(\Sigma \times (-a, a))$ coincides with $\Omega$ defined by (3). In other words, $\Omega$ is a submanifold of $\mathbb{R}^3$ squeezed between two parallel surfaces at the distance $a$ from $\Sigma$.

Using (7), we can identify $\Omega$ with the Riemannian manifold $\Sigma \times (-a, a)$ endowed with the metric $G$ induced by $\mathcal{L}$. One has
\[
G(x, u) = g(x) \circ (I_x - L_x u)^2 + du^2,
\]
where $I_x$ denotes the identity map on $T_x \Sigma$. By the definition of principal curvatures, it is easy to see that the measure on $\Omega \simeq (\mathbb{R} \times (-a, a), G)$ at a point $(x, u)$ acquires the form
\[
d\Omega = (1 - k_1(x) u)(1 - k_2(x) u) d\Sigma du,
\]
where $d\Sigma du$ stands for the product measure on $\Sigma \times (-a, a)$ at $(x, u)$. Here $d\Sigma = |g(x)|^{1/2} dx^1 dx^2$ in a local coordinate system of $\Sigma$ at $x$, with the usual notation $|g| := \det(g)$.

Let $G^{ij}$ be the coefficients of the inverse of $G$ in local coordinates $(x, u)$ for $\Sigma \times (-a, a)$. Using the above identification, $-\Delta_{D}$ is unitarily equivalent to the self-adjoint operator $H$ associated with the quadratic form $h$ defined in the Hilbert space $\mathcal{H} := L^2(\Sigma \times (-a, a), d\Omega)$ by
\[
h[\Psi] := \int_{\Sigma \times (-a, a)} (\partial_j \Psi(x, u)) G^{ij}(x, u) (\partial_i \Psi(x, u)) d\Omega,
\]
for $\Psi \in \text{Dom } h := W^{1, 2}_{0, 2}(\Sigma \times (-a, a), d\Omega)$.

Here the Sobolev space $W^{1, 2}_{0, 2}(\Sigma \times (-a, a), d\Omega)$ is defined as the completion of functions from $C_0^\infty(\Sigma \times (-a, a))$ with respect to the norm $(h[.] + \|\cdot\|_2^2)^{1/2}$. Consequently, to prove Theorem 1 it is equivalent to establish the lower bound (14) for the operator $H$.

Proof of Theorem 2. Let $\Psi$ be any function defined in $C_0^\infty(\Sigma \times (-a, a))$, a dense subspace of $\text{Dom } h$. Since $(G^{\mu\nu})_{\mu, \nu=1, 2}$ is positive definite, one has
\[
h[\Psi] \geq \int_{\Sigma} d\Sigma \int_{-a}^{a} du \left| \partial_u \Psi(x, u) \right|^2 \left( 1 - k_1(x) u \right) \left( 1 - k_2(x) u \right)
\geq \int_{\Sigma} d\Sigma \lambda_1(k_1(x), k_2(x)) \int_{-a}^{a} du \left| \Psi(x, u) \right|^2 \left( 1 - k_1(x) u \right) \left( 1 - k_2(x) u \right),
\]
where \( \lambda_1(\kappa_1, \kappa_2) \) is defined by (5). It remains to show that
\[
\lambda_1(k_1(x), k_2(x)) \geq \min \{ \lambda_1(k_1^+, k_2^-), \lambda_1(k_1^-, k_2^+) \} \tag{12}
\]
for all \( x \in \Sigma \). Given constants \( \kappa_1, \kappa_2 \in (-1/a, 1/a) \), the change of test function \( \phi := \sqrt{(1 - \kappa_1 u)(1 - \kappa_2 u)} \psi \) in (5) and an integration by parts yields
\[
\lambda_1(\kappa_1, \kappa_2) = \inf_{\phi \in W_0^{1,2}((-a,a)) \setminus \{0\}} \frac{\int_a^{-a} (|\phi''(u)|^2 + V(u; \kappa_1, \kappa_2) |\phi(u)|^2) \, du}{\int_a^{-a} |\phi(u)|^2 \, du}, \tag{13}
\]
where
\[
V(u; \kappa_1, \kappa_2) := -\frac{1}{4} \frac{(\kappa_1 - \kappa_2)^2}{(1 - \kappa_1 u)^2(1 - \kappa_2 u)^2}. \tag{14}
\]
The constant lower bound (12) then follows by observing that
\[
V(u; k_1(x), k_2(x)) \geq \min \{ V(u; k_1^+, k_2^-), V(u; k_1^-, k_2^+) \}
\]
for any fixed \( u \in (-a, a) \) and all \( x \in \Sigma \). The last inequality can be established for non-zero \( u \)'s by writing
\[
V(u; \kappa_1, \kappa_2) = -\frac{1}{4u^2} \left[ \frac{1}{(1 - \kappa_1 u)} - \frac{1}{(1 - \kappa_2 u)} \right]^2 \tag{15}
\]
and follows more easily for \( u = 0 \).

**Remark 1.** Following [3, Rem. 1], since the hypothesis (2) is still enough to ensure that \( (\Sigma \times (-a,a), G) \) is immersed in \( \mathbb{R}^3 \), we do not need to assume (8) in order to get (11) for the operator \( H \).

Let us now derive the uniform lower bound of Proposition 1.

**Proof of Proposition 1.** In view of (5), without loss of generality we may assume that \( \kappa_1 \) and \( \kappa_2 \) are non-negative. By (13) with (15), we have
\[
\lambda_1(\kappa_1, \kappa_2) \geq \min\{\lambda_1(\kappa_1, 0), \lambda_1(0, \kappa_2)\}.
\]

However, \( \lambda_1(\kappa, 0) = \lambda_1(0, \kappa) \) with \( \kappa \in [0, 1/a) \) is the spectral threshold of the Dirichlet Laplacian in the strip of cross-section \((-a, a)\) built either over a circle of curvature \( \kappa \) if \( \kappa \neq 0 \) or over a straight line if \( \kappa = 0 \). With help of monotonicity properties established in [5, Prop. 4.2] (or using again (13) with (15)), the Faber-Krahn inequality yields (cf [5, Prop. 4.5])
\[
\lambda_1(0, \kappa) \geq j_{0,1}^2/(2a)^2
\]
for all \( \kappa \in [0, 1/a) \). Notice that \( \lambda_1(0, 1/a) \) is the lowest eigenvalue of the Dirichlet Laplacian in the disk of radius \( 2a \).
Finally, we establish Proposition 2.

Proof of Proposition 2. For any positive number $\varepsilon < \min\{1, a\}$, let us set

$$\psi_\varepsilon(u) := \begin{cases} 1 & \text{if } |u| \leq a - \varepsilon, \\ -\frac{\log((a - u)/\varepsilon^2)}{\log(\varepsilon)} & \text{if } a - \varepsilon \leq |u| \leq a - \varepsilon^2 \\ 0 & \text{if } a - \varepsilon^2 \leq |u|. \end{cases}$$

Then $\psi_\varepsilon \in W^{1,2}_0((-a, a))$ and using $\psi_\varepsilon$ as a test function in the right hand side of (5) with $\kappa_1 := -1/a$ and $\kappa_2 := 1/a$, we obtain

$$\lambda_1(-1/a, 1/a) \leq 2 \int_0^a |\psi_\varepsilon'(u)|^2 (1 - u/a) \, du \int_0^a |\psi_\varepsilon(u)|^2 (1 - u/a) \, du,$$

where we used the bounds $1 \leq 1 + u/a \leq 2$. While the denominator converges to $\int_0^a (1 - u/a) \, du = a/2$, an explicit computation shows that the numerator tends to zero as $\varepsilon \to 0$. \hfill \qed

Remark 2. Note that (13) yields a Hardy-Poincaré-type inequality

$$\int_{-\kappa}^{\kappa} |\phi'(u)|^2 \, du \geq \lambda_1(\kappa_1, \kappa_2) \int_{-\kappa}^{\kappa} |\phi(u)|^2 \, du + \int_{-\kappa}^{\kappa} |V(u; \kappa_1, \kappa_2)| |\phi(u)|^2 \, du \quad (16)$$

for all $\phi \in W^{1,2}_0((-\kappa, \kappa))$ and $\kappa_1, \kappa_2 \in [-1/a, 1/a]$, where the Hardy weight $V(\cdot; \kappa_1, \kappa_2)$ is given by (14) and the Poincaré constant $\lambda_1(\kappa_1, \kappa_2)$ interpolates between 0 and $\pi^2/(2a)^2$. An equivalent version of this inequality in weighted spaces follows from (5). If $\kappa_1 = \kappa_2 = 0$, then $V(\cdot; \kappa_1, \kappa_2)$ vanishes identically and $\lambda_1(\kappa_1, \kappa_2)$ equals $\pi^2/(2a)^2$, the first eigenvalue of the Dirichlet Laplacian in the interval $(-a, a)$. On the other hand, putting $\kappa_1 = 1/a$ and $\kappa_2 = -1/a$ in (16), Proposition 2 yields an optimal Hardy-type inequality

$$\int_{-\kappa}^{\kappa} |\phi'(u)|^2 \, du \geq \int_{-\kappa}^{\kappa} \frac{a^2}{(a^2 - u^2)^2} |\phi(u)|^2 \, du \quad (17)$$

for all $\phi \in W^{1,2}_0((-\kappa, \kappa))$. We remark that this inequality is better than the well-known bound (see, e.g., (11))

$$\int_{-\kappa}^{\kappa} |\phi'(u)|^2 \, du \geq \int_{-\kappa}^{\kappa} \frac{1}{4(a - |u|)^2} |\phi(u)|^2 \, du$$

for all $\phi \in W^{1,2}_0((-\kappa, \kappa))$, which can be established by the classical Hardy inequality. Notice that the function $a - |\cdot|$ has the meaning of the distance to the boundary of the one-dimensional domain $(-a, a)$. Hardy inequalities with weights of type (14) have been recently considered for higher-dimensional domains in (4) (see also (2) Lem. 8)).
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Pedro Freitas, Department of Mathematics, Faculty of Human Kinetics & Group of Mathematical Physics, Faculdade de Ciências da Universidade de Lisboa, Campo Grande, Edifício C6 1749-016 Lisboa, Portugal
E-mail: psfreitas@fc.ul.pt

David Krejčiřík, Department of Theoretical Physics, Nuclear Physics Institute, Academy of Sciences, 25068 Řež, Czech Republic
E-mail: krejcirik@ujf.cas.cz