Trapped modes in finite quantum waveguides

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Abstract. The Laplace operator in infinite quantum waveguides (e.g., a bent strip
or a twisted tube) often has a point-like eigenvalue below the essential spectrum that
 corresponds to a trapped eigenmode of finite L2 norm. We revisit this statement for
resonators with long but finite branches that we call “finite waveguides”. Although
now there is no essential spectrum and all eigenfunctions have finite L2 norm, the
trapping can be understood as an exponential decay of the eigenfunction inside the
branches. We describe a general variational formalism for detecting trapped modes
in such resonators. For finite waveguides with general cylindrical branches, we obtain
a sufficient condition which determines the minimal length of branches for getting
a trapped eigenmode. Varying the branch lengths may switch certain eigenmodes
from non-trapped to trapped states. These concepts are illustrated for several typical
waveguides (L-shape, bent strip, crossing of two stripes, etc.). We conclude that
the well-established theory of trapping in infinite waveguides may be incomplete and
require further development for being applied to microscopic quantum devices.

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1. Introduction

By its name, a waveguide serves for propagating waves which may be of different physical origins: fluctuations of pressure in acoustics, electromagnetic waves in optics, particle waves in quantum mechanics, surface water waves in hydrodynamics, etc. The transmission properties of a waveguide can be characterized by its resonance frequencies or, equivalently, by the spectrum of an operator which describes the waves motion (e.g., the Laplace operator in the most usual case). For infinite waveguides, the spectrum consists of two parts: (i) the essential (or continuous) spectrum for which the related resonances are extended over the whole domain and thus have infinite $L_2$ norms, and (ii) the discrete (or point-like) spectrum for which the related eigenfunctions have finite $L_2$ norms and thus necessarily “trapped” or “localized” in a region of the waveguide. A wave excited at the frequency of the trapped eigenmode remains in the localization region and does not propagate.

The existence of trapped, bound or localized eigenmodes in classical and quantum waveguides has been thoroughly investigated (see reviews [1, 2] and also references in [3]). In the seminal paper, Rellich proved the existence of a localized eigenfunction in a deformed infinite cylinder [4]. His results were significantly extended by Jones [5]. Ursell reported on the existence of trapped modes in surface water waves in channels [6, 7, 8], while Parker observed experimentally the trapped modes in locally perturbed acoustic waveguides [9, 10]. Exner and Seba considered an infinite bent strip of smooth curvature and showed the existence of trapped modes by reducing the problem to Schrödinger operator in the straight strip, with the potential depending on the curvature [11]. Goldstone and Jaffe gave the variational proof that the wave equation subject to Dirichlet boundary condition always has a localized eigenmode in an infinite tube of constant cross-section in any dimension, provided that the tube is not exactly straight [12]. The problem of localization in acoustic waveguides with Neumann boundary condition has also been investigated [13, 14]. For instance, Evans et al. considered a straight strip with an inclusion of arbitrary (but symmetric) shape [14] (see [15] for further extension). Such an inclusion obstructed the propagation of waves and was shown to result in trapped modes. The effect of mixed Dirichlet, Neumann and Robin boundary conditions on the localization was also investigated (see [3, 16] and references therein). A mathematical analysis of guided water waves was developed in [17].

All the aforementioned works dealt with infinite waveguides for which the Laplace operator spectrum is essential, with possible inclusion of discrete points. Since these discrete points were responsible for trapped modes, the major question was whether or not such discrete points exist below the essential spectrum. It is worth noting that the localized modes have to decay relatively fast at infinity in order to guarantee the finite $L_2$ norm. But the same question about the existence of rapidly decaying eigenfunctions may be formulated for bounded domains (resonators) with long branches that we call “finite waveguides” (Fig. 1). This problem is different in many aspects. Since all eigenfunctions have now finite $L_2$ norms, the definition of trapped or localized modes has to be revised.
Quite surprisingly, a rigorous definition of localization in bounded domains turns out to be a challenging problem \[18, 19, 20\]. In the context of the present paper concerning finite waveguides, an eigenmode is called trapped or localized if it decays exponentially fast in prominent subregions (branches) of the bounded domain. The exponential decay of an eigenfunction in the branch can be related to the smallness of the associated eigenvalue in comparison to the cut-off frequency, i.e. the first eigenvalue of the Laplace operator in the cross-section of that branch \[21\]. In other words, the existence of a trapped mode is related to “smallness” of the eigenvalue, in full analogy to infinite waveguides. Using the standard mathematical tools such as domain decomposition, explicit representation of solutions of the Helmholtz equation and variational principle, we aim at formalizing these ideas and providing a sufficient condition on the branch lengths for getting a trapped mode. The dependence of the localization character on the length of branches is the main result of the paper and a new feature of finite waveguides which was overseen in the well-established theory of infinite waveguides. As in practice all quantum waveguides are finite, this dependence may be important for microelectronic devices.

The paper is organized as follows. In Sec. 2 we adapt the method by Bonnet-Ben Dhia and Joly \[17\] in order to reduce the original eigenvalue problem in the whole domain to the nonlinear eigenvalue problem in the domain without branches. Although the new problem is more sophisticated, its variational reformulation provides a general framework for proving the trapping (or localization) of eigenfunctions. We use it to derive the main result of the paper: a sufficient condition \([19]\) on the branch lengths for getting a trapped mode. In sharp contrast to an infinite (non-straight) waveguide of a constant cross-section, for which the first eigenfunction is always trapped and exponentially decaying \([12]\), finite waveguides may or may not have such an eigenfunction, depending on the length of branches. This method is then illustrated in Sec. 3 for several finite waveguides (e.g., a bent strip and a cross of two stripes). For these examples, we estimate the minimal branch length which is sufficient for getting at least one localized mode. At the same time, we provide an example of a waveguide, for which there is no localization for any branch length. We also construct a family of finite waveguides for which the minimal branch length varies continuously. As a consequence, for a given (large enough) branch length, one can construct two almost identical resonators, one with and the other without localized mode. This observation may be used for developing quantum switching devices.

2. Theoretical results

For the sake of clarity, we focus on planar bounded domains with rectangular branches, while the extension to arbitrary domains in \(\mathbb{R}^n\) with general cylindrical branches is straightforward and provided at the end of this Section.

We consider a planar bounded domain \(D\) composed of a basic domain \(\Omega\) of arbitrary
shape and $M$ rectangular branches $Q_i$ of lengths $a_i$ and width $b$ as shown on Fig. 1.

$$D = \Omega \cup \bigcup_{i=1}^{M} Q_i.$$  

We denote $\Gamma_i = \partial \Omega \cap \partial Q_i$ the inner boundary between the basic domain $\Omega$ and the branch $Q_i$ and $\Gamma = \partial \Omega \setminus \bigcup_{i=1}^{M} \Gamma_i$ the exterior boundary of $\Omega$. We study the eigenvalue problem for the Laplace operator with Dirichlet boundary condition

$$-\Delta U = \lambda U, \quad U|_{\partial D} = 0. \quad (1)$$

### 2.1. Solution in rectangular branches

Let $u_i(x, y)$ denote the restriction of the solution $U(x, y)$ of the eigenvalue problem (1) to the branch $Q_i$. For convenience, we take $b = 1$ and assume that the coordinates $x$ and $y$ are chosen in such a way that $Q_i = \{(x, y) \in \mathbb{R}^2 : 0 < x < a_i, 0 < y < 1\}$ (the final result will not depend on this particular coordinate system). The eigenfunction $u_i(x, y)$ satisfying Dirichlet boundary condition on $\partial Q_i$ has the standard representation:

$$u_i(x, y) \equiv U|_{Q_i} = \sum_{n=1}^{\infty} c_n \sinh(\gamma_n(a_i - x)) \sin(\pi ny), \quad (2)$$

where $\gamma_n = \sqrt{\pi^2 n^2 - \lambda}$ and $c_n$ are the Fourier coefficients of the function $U$ at the inner boundary $\Gamma_i$ (at $x = 0$):

$$c_n = \frac{2}{\sinh(\gamma_n a_i)} \int_{0}^{1} dy \ U(0, y) \sin(\pi ny). \quad (3)$$

Substituting this relation into Eq. (2) yields

$$u_i(x, y) = 2 \sum_{n=1}^{\infty} (U|_{\Gamma_i} \sin(\pi ny))_{L_2(\Gamma_i)} \frac{\sinh(\gamma_n(a_i - x))}{\sinh(\gamma_n a_i)} \sin(\pi ny), \quad (4)$$

where the integral in (3) was interpreted as the scalar product in $L_2(\Gamma_i)$. The representation (4) is of course formal because its coefficients are still unknown. Nevertheless, one can already distinguish two different cases.
(i) If $\lambda < \frac{\pi}{2}$, all $\gamma_n$ are real, and the representation (1) decays exponentially. In fact, writing the squared $L_2$-norm of the function $u_i(x, y)$ along the vertical cross-section of the branch $Q_i$ at $x$,

$$I_i(x) \equiv \int_0^1 u_i^2(x, y) dy = 2 \sum_{n=1}^{\infty} (U_{|\Gamma_i}, \sin(\pi ny))_{L_2(\Gamma_i)}^2 \frac{\sinh^2(\gamma_n(a_i - x))}{\sinh^2(\gamma_n a_i)},$$

one can use the inequality $\sinh(\gamma_n(a_i - x)) \leq \sinh(\gamma_n a_i) e^{-\gamma_1 x}$ to get

$$I_i(x) \leq 2 \sum_{n=1}^{\infty} (U_{|\Gamma_i}, \sin(\pi ny))_{L_2(\Gamma_i)}^2 e^{-2\gamma_1 x} = I_i(0) e^{-2\gamma_1 x} \quad (0 < x < a_i). \quad (5)$$

This shows the exponential decay along the branch with the decay rate $2\gamma_1 = 2\sqrt{\pi^2 - \lambda}$.

(ii) In turn, if $\lambda > \frac{\pi}{2}$, some $\gamma_n$ are purely imaginary so that $\sinh(\gamma_n z)$ becomes $\sin(|\gamma_n| z)$, and the exponential decay is replaced by an oscillating behavior.

One sees that the problem of localization of the eigenfunction in the basic domain $\Omega$ is reduced to checking whether the eigenvalue $\lambda$ is smaller or greater than $\frac{\pi}{2}$ (or $\frac{\pi}{2}/b^2$ in general).

### 2.2. Nonlinear eigenvalue problem

The explicit representation (1) of the eigenfunction in the branch $Q_i$ allows one to reformulate the original eigenvalue problem (1) in the whole domain $D$ as a specific eigenvalue problem in the basic domain $\Omega$. In fact, the restriction of $U$ onto the basic domain $\Omega$, $u \equiv U|\Omega$, satisfies the following equations

$$-\Delta u = \lambda u \quad \text{in } \Omega, \quad u|_{\Gamma} = 0, \quad u|_{\Gamma_i} = u_i|_{\Gamma_i}, \quad \frac{\partial u}{\partial n}|_{\Gamma_i} = -\frac{\partial u_i}{\partial n}|_{\Gamma_i}, \quad (6)$$

where $\partial/\partial n$ denotes the normal derivative directed outwards the domain. The last two conditions ensure that the eigenfunction and its derivative are continuous at inner boundaries $\Gamma_i$ (the sign minus accounting for opposite orientations of the normal derivatives on both sides of the inner boundary). The normal derivative of $u_i$ can be explicitly written by using Eq. (4):

$$\frac{\partial u_i}{\partial n}|_{\Gamma_i} = -\frac{\partial u_i}{\partial x}|_{x=0} = 2 \sum_{n=1}^{\infty} \gamma_n \coth(\gamma_n a_i) (U_{|\Gamma_i}, \sin(\pi ny))_{L_2(\Gamma_i)} \sin(\pi ny). \quad (7)$$

Denoting $T_i(\lambda)$ an operator acting from $H^{1/2}(\Gamma_i)$ to $H^{-1/2}(\Gamma_i)$ (see [22] for details) as

$$T_i(\lambda) f \equiv 2 \sum_{n=1}^{\infty} \gamma_n \coth(\gamma_n a_i) (f, \sin(\pi ny))_{L_2(\Gamma_i)} \sin(\pi ny),$$

the right-hand side of Eq. (7) can be written as

$$\frac{\partial u_i}{\partial n}|_{\Gamma_i} = T_i(\lambda) U_{|\Gamma_i}.$$ 

The eigenvalue problem (6) admits thus a closed representation as

$$-\Delta u = \lambda u \quad \text{in } \Omega, \quad u|_{\Gamma} = 0, \quad \frac{\partial u}{\partial n}|_{\Gamma_i} = -T_i(\lambda) u_{|\Gamma_i}. \quad (8)$$
The presence of branches and their shapes are fully accounted for by the operators $T_i$ which are somewhat analogous to Dirichlet-to-Neumann operators.

Although this domain decomposition allows one to remove the branches and get a closed formulation for the basic domain $\Omega$, the new eigenvalue problem is nonlinear because the eigenvalue $\lambda$ appears also in the boundary condition through the operators $T_i(\lambda)$. A trick to overcome this difficulty goes back to the Birman-Schwinger method [23, 24] (see also [25]). Following [17], we fix $\lambda$ and solve the linear eigenvalue problem

$$-\Delta u = \mu(\lambda) u \quad \text{in } \Omega, \quad u|_{\Gamma} = 0, \quad \frac{\partial u}{\partial n}|_{r_i} = - T_i(\lambda) u|_{r_i},$$

(9)

where $\mu(\lambda)$ denotes the eigenvalue which is parameterized by $\lambda$. The solution of the original problem is recovered when $\mu(\lambda) = \lambda$.

From a practical point of view, a numerical solution of Eqs. (9) with the subsequent resolution of the equation $\mu(\lambda) = \lambda$ is in general much more difficult than solving the original eigenvalue problem (see also [26] for possible numerical schemes). In turn, Eqs. (9) are convenient for checking whether the first eigenvalue $\lambda_1$ is smaller or greater than $\pi^2$, as explained below.

2.3. Variational formulation

We search for a weak solution of the eigenvalue problem (9) in the Sobolev space

$$H^1_0(\Omega) = \{v(x, y) \in L^2(\Omega), \partial v/\partial x \in L^2(\Omega), \partial v/\partial y \in L^2(\Omega), \text{ } v|_{\Gamma} = 0\}.$$

Multiplying Eq. (9) by a trial function $v \in H^1_0(\Omega)$ and integrating by parts, one gets

$$\mu(\lambda) \int_\Omega vu = - \int_\Omega v \Delta u = \int_\Omega (\nabla v, \nabla u) - \int_{\partial \Omega} v \frac{\partial u}{\partial n}.$$

Since $v$ vanishes on $\Gamma$, the weak formulation of the problem reads as

$$(\nabla u, \nabla v)_{L^2(\Omega)} + \sum_{i=1}^M (T_i(\lambda) u, v)_{L^2(\Gamma_i)} = \mu(\lambda)(u, v)_{L^2(\Omega)} \quad \forall v \in H^1_0(\Omega).$$

(10)

The first eigenvalue $\mu_1(\lambda)$ is then obtained from the Rayleigh’s principle

$$\mu_1(\lambda) = \inf_{v \in H^1_0(\Omega), \ v \neq 0} \frac{(\nabla v, \nabla v)_{L^2(\Omega)} + \sum_{i=1}^M (T_i(\lambda) v, v)_{L^2(\Gamma_i)}}{(v, v)_{L^2(\Omega)}}.$$  

(11)

One can show that $\mu_1(\lambda)$ is a continuous monotonously decreasing function of $\lambda$ on the segment $(0, \pi^2]$. For this purpose, one first computes explicitly the derivative of the function

$$h(\lambda) \equiv \gamma_n \coth(\gamma_n a_i) = \sqrt{\pi^2 n^2 - \lambda} \coth(\sqrt{\pi^2 n^2 - \lambda} a_i)$$

and checks that $h'(\lambda) < 0$. Now one can show that $\mu_1(\lambda_1) \leq \mu_1(\lambda_2)$ if $\lambda_1 > \lambda_2$. If some trial function $v_2$ minimizes the Rayleigh’s quotient (11) for $\lambda_2$, one has

$$\mu_1(\lambda_1) \leq \frac{(\nabla v_2, \nabla v_2)_{L^2(\Omega)} + \sum_{i=1}^M (T_i(\lambda_1) v_2, v_2)_{L^2(\Gamma_i)}}{(v_2, v_2)_{L^2(\Omega)}} \leq \frac{(\nabla v_2, \nabla v_2)_{L^2(\Omega)} + \sum_{i=1}^M (T_i(\lambda_2) v_2, v_2)_{L^2(\Gamma_i)}}{(v_2, v_2)_{L^2(\Omega)}} = \mu_1(\lambda_2),$$

(11)
where the monotonous decrease of the function $h(\lambda)$ was used (the mathematical proof of the continuity for an analogous functional is given in [27]).

Since the function $\mu_1(\lambda)$ is positive, continuous and monotonously decreasing, the equation $\mu_1(\lambda) = \lambda$ has a solution $0 < \lambda < \pi^2$ if and only if $\mu_1(\pi^2) < \pi^2$. This is a necessary and sufficient condition for getting a trapped mode for the linear eigenvalue problem (9).

2.4. Sufficient condition

For any trial function $v \in H_0^1(\Omega)$, we denote the Rayleigh’s quotient

$$
\mu(v) = \frac{(\nabla v, \nabla v)_{L^2(\Omega)} + \sum_{i=1}^{M} (T_i(\pi^2)v, v)_{L^2(\Gamma_i)}}{(v, v)_{L^2(\Omega)}}. \quad (12)
$$

Since $\gamma_n(\pi^2) = \pi\sqrt{n^2 - 1}$, one has $\gamma_1(\pi^2) = 0$, and the operators $T_i(\pi^2)$ can be decomposed into two parts so that

$$
\mu(v) = (v, v)_{L^2(\Omega)}^{-1} \left\{ (\nabla v, \nabla v)_{L^2(\Omega)} + 2 \sum_{i=1}^{M} \frac{1}{a_i} (v, \sin(\pi y))^2_{L^2(\Gamma_i)} 
+ 2\pi \sum_{n=2}^{\infty} \sqrt{n^2 - 1} \sum_{i=1}^{M} \coth(\pi a_i \sqrt{n^2 - 1}) (v, \sin(\pi ny))^2_{L^2(\Gamma_i)} \right\}. \quad (13)
$$

If one finds a trial function $v \in H_0^1(\Omega)$ for which $\mu(v) < \pi^2$, then the first eigenvalue $\mu_1(\pi^2)$ necessarily satisfies this condition because $\mu_1(\pi^2) \leq \mu(v)$. The inequality $\mu(v) < \pi^2$ is thus a sufficient (but not necessary) condition. Given that $\coth(\pi a_i \sqrt{n^2 - 1}) \leq \coth(\pi a_i \sqrt{3})$ for any $n \geq 2$, the sufficient condition can be written as

$$
\sum_{i=1}^{M} \frac{\sigma_i}{a_i} < \beta - \sum_{i=1}^{M} \kappa_i \coth(\pi a_i \sqrt{3}), \quad (14)
$$

where

$$
\beta = \pi^2 (v, v)_{L^2(\Omega)} - (\nabla v, \nabla v)_{L^2(\Omega)}, \quad (15)
$$
$$
\sigma_i = 2(v, \sin(\pi y))^2_{L^2(\Gamma_i)}, \quad (16)
$$
$$
\kappa_i = 2\pi \sum_{n=2}^{\infty} \sqrt{n^2 - 1} (v, \sin(\pi ny))^2_{L^2(\Gamma_i)}. \quad (17)
$$

Before moving to examples, several remarks are in order.

(i) The shape of the branches enters through the operator $T_i(\lambda)$. Although the above analysis was presented for rectangular branches, its extension to bounded domains in $\mathbb{R}^n$ with general cylindrical branches is straightforward and based on the variable separation (in directions parallel and perpendicular to the branch). In fact, the Fourier coefficients $(u, \sin(\pi ny))_{L^2(\Gamma_i)}$ on the unit interval (i.e., the cross-section of the rectangular branch) have to be replaced by a spectral decomposition over the orthonormal eigenfunctions $\{\psi_n(y)\}_{n=1}^{\infty}$ of the Laplace operator $\Delta_\perp$ in the cross-section $\Gamma_i$ of the studied branch (in general, $\Gamma_i$ is a bounded domain in $\mathbb{R}^{n-1}$):

$$
\Delta_\perp \psi_n + \nu_n \psi_n = 0 \quad \text{in} \quad \Gamma_i, \quad \psi_n|_{\partial \Gamma_i} = 0. \quad (18)
$$
In particular, the operator $T_i(\lambda)$ becomes

$$T_i(\lambda)f = \sum_{n=1}^{\infty} \gamma_n \coth(\gamma_n a_i)(f, \psi_n)_{L_2(\Gamma_i)} \psi_n(y),$$

with $\gamma_n = \sqrt{\nu_n - \lambda}$. Repeating the above analysis, one immediately deduces a sufficient condition for getting a trapped mode:

$$\sum_{i=1}^{M} \frac{\sigma_i}{a_i} < \beta - \sum_{i=1}^{M} \kappa_i \coth(a_i \sqrt{\nu_2 - \nu_1}),$$

(19)

with

$$\beta = \nu_1(v, v)_{L_2(\Omega)} - (\nabla v, \nabla v)_{L_2(\Omega)},$$

(20)

$$\sigma_i = (v, \psi_1)^2_{L_2(\Gamma_i)},$$

(21)

$$\kappa_i = \sum_{n=2}^{\infty} \sqrt{\nu_n - \nu_1} (v, \psi_n)^2_{L_2(\Gamma_i)},$$

(22)

One retrieves the above results for rectangular branches by putting $\psi_n(y) = \sqrt{2} \sin(\pi n y)$ and $\nu_n = \pi^2 n^2$.

The inequality (19) is the main result of the paper. Although there is no explicit recipe for choosing the trial function $v$ (which determines the coefficients $\beta$, $\sigma_i$ and $\kappa_i$), this is a general framework for studying the localization (or trapping) in domains with cylindrical branches.

(ii) If the branches are long enough (e.g., $a_i \gg (\nu_2 - \nu_1)^{-1/2}$), the values $\coth(a_i \sqrt{\nu_2 - \nu_1})$ are very close to 1 and can be replaced by $1 + \epsilon$ where $\epsilon$ is set by the expected minimal length so that the inequality (19) becomes more explicit in terms of $a_i$:

$$\sum_{i=1}^{M} \frac{\sigma_i}{a_i} < \beta - (1 + \epsilon) \sum_{i=1}^{M} \kappa_i,$$

(23)

In the particular case when all $\sigma_i$ are the same, one can introduce the threshold value $\eta$ as

$$\sum_{i=1}^{M} \frac{1}{a_i} < \eta, \quad \eta \equiv \frac{\beta}{\sigma_1} - \frac{(1 + \epsilon)}{\sigma_1} \sum_{i=1}^{M} \kappa_i.$$  

(24)

For domains with identical branches, $a_i = a$, the above condition determines the branch length $a_{th} = M/\eta$ which is long enough for the emergence of localization. This means that for any $a > a_{th}$, there is a localized eigenmode. Since $a_{th}$ was obtained from the sufficient condition (19), the opposite statement is not true: for $a < a_{th}$, this condition does not indicate whether the eigenfunction is localized or not. In fact, $a_{th}$ is the upper bound for the minimal branch length $a_{min}$ which may distinguish waveguides with and without localized modes (see Sec. 3).

(iii) The trial function should be chosen to ensure the convergence of the series in (22). If the boundary of $\Omega$ is smooth, the series in (22) converges for any function $v$ from
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$H_0^1(\Omega)$ according to the trace theorem \[22\]. In turn, the presence of corners or other singularities may require additional verifications for the convergence, as illustrated in Sec. 3.3.

(iv) The implementation of various widths $b_i$ of the rectangular branches is relatively straightforward (e.g., $\sin(\pi ny)$ is replaced by $\sin(\pi ny/b_i)$, etc.). In order to guarantee the exponential decay in all branches, one needs $\lambda < \pi^2/b_i^2$ for all $i$, i.e., $\lambda < \pi^2/\max\{b_i^2\}$. Rescaling the whole domain in such a way that $\max\{b_i\} = 1$, one can use the above conditions.

(v) According to Eq. (5), the decay rate, $2\gamma_1$, is determined by the eigenvalue $\lambda$. Since $\mu(v)$ is an upper bound for the first eigenvalue, one gets a lower bound for the decay rate:

$$2\gamma_1 \geq 2\sqrt{\nu_1 - \mu(v)} = 2(v,v)^{-1/2}_{L_2(\Omega)} \left( \beta - \sum_{i=1}^{M} [\sigma_i/a_i + \kappa_i \coth(a_i\sqrt{\nu_2 - \nu_1})] \right)^{1/2}.$$

3. Several examples

As we already mentioned, there is no general recipe for choosing a trial function $v$ from $H_0^1(\Omega)$. Of course, the best possible choice is the eigenfunction on which $\mu(v)$ reaches its minimum. Except for few cases, the eigenfunction is not known but one can often guess how it behaves for a given basic domain. Since the gradient of the trial function $v$ enters into the coefficient $\beta$ with the sign minus, slowly varying functions are preferred. In what follows, we illustrate these concepts for several examples.

3.1. L-shape

We start by a classical problem of localization in L-shape with two rectangular branches of lengths $a_1$ and $a_2$ (Fig. 2a) for which the basic domain is simply the unit square. In the limit case $a_1 = a_2 = 0$ (i.e., $D = \Omega$, without branches), the first eigenvalue $\lambda_1 = 2\pi^2 > \pi^2$ so that, according to our terminology, there is no localization. Since $\lambda_1$ continuously varies with $a$ ($a_1 = a_2 = a$), the inequality $\lambda_1 > \pi^2$ also remains true for

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**Figure 2.** Three types of a bent waveguide: (a) L-shape, (b) bent strip, and (c) truncated L-shapes parameterized by the length $\ell$ varying from 0 (triangular basic domain) to 1 (the original L-shape).
relatively short branches. In turn, given that \( \lambda < \pi^2 \) for infinitely long branches, there should exist the minimal branch length \( a_{\text{min}} \) such that \( \lambda = \pi^2 \). At this length, the first eigenfunction passes from non-localized state \((a < a_{\text{min}})\) to localized state \((a > a_{\text{min}})\). In what follows, we employ the sufficient condition (14) in order to get the upper bound for \( a_{\text{min}} \).

The most intuitive choice for the trial function would be the first eigenfunction for the unit square with Dirichlet boundary condition,

\[
v(x, y) = \sin(\pi x) \sin(\pi y).
\]

However, one easily checks that \( \beta = 0 \) for this function, while \( \sigma_i \) and \( \kappa_i \) are always non-negative. As a consequence, the condition (14) is never satisfied for this trial function. It simply means that the first choice was wrong.

For the trial function

\[
v(x, y) = (1 + x) \sin(\pi y) + (1 + y) \sin(\pi x),
\]

the explicit integration yields

\[
(v, v)_{L_2(\Omega)} = \int_{-1}^{0} dx \int_{-1}^{0} dy [(1 + x) \sin(\pi y) + (1 + y) \sin(\pi x)]^2 = \frac{1}{3} + \frac{2}{\pi^2},
\]

\[
(\nabla v, \nabla v)_{L_2(\Omega)} = \int_{-1}^{0} dx \int_{-1}^{0} dy \left[ \left( \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right] = \frac{\pi^2}{3} + 1,
\]

\[
(v, \sin(\pi y))_{L_2(\Gamma_1)} = \int_{-1}^{0} dy [(1 + 0) \sin(\pi y) + (1 + y) \sin(\pi 0)] \sin(\pi y) = \frac{1}{2},
\]

\[
(v, \sin(\pi ny))_{L_2(\Gamma_1)} = (v, \sin(\pi nx))_{L_2(\Gamma_2)} = 0 \quad (n \geq 2).
\]

from which

\[
\beta = 1, \quad \sigma_1 = \sigma_2 = \frac{1}{2}, \quad \kappa_1 = \kappa_2 = 0.
\]

The condition (14) reads as

\[
\frac{1}{a_1} + \frac{1}{a_2} < 2.
\]

If the branches have the same length, \( a_1 = a_2 = a \), then the upper bound of the minimal branch length for getting a localized eigenfunction is given by \( a_{\text{th}} = 1 \).

We also solved the original eigenvalue problem (1) for L-shape with \( a_1 = a_2 = a \) by a finite element method (FEM) implemented in Matlab PDEtools. The first eigenvalue \( \lambda_1 \) as a function of the branch length \( a \) is shown by solid line on Fig. 3. One can clearly see a transition from non-localized \((\lambda_1 > \pi^2)\) to localized \((\lambda_1 < \pi^2)\) states when \( a \) crosses the minimal branch length \( a_{\text{min}} \approx 0.84 \). As expected, the theoretical upper bound \( a_{\text{th}} \), which was obtained from a sufficient condition, exceeds the numerical value \( a_{\text{min}} \). In order to improve the theoretical estimate, one has to search for trial functions which are closer to the true eigenfunction. At the same time, \( a_{\text{th}} \) and \( a_{\text{min}} \) are close to each other, and the accuracy of the theoretical result is judged as good. Similar results for L-shape in three dimensions are derived in Appendix A.
Figure 3. The first eigenvalue $\lambda_1$ divided by $\pi^2$, as a function of the branch length $a$ ($a_1 = a_2 = a$), for three bent waveguides shown on Fig. 2: L-shape (solid line), bent strip (dashed line) and truncated L-shape with $\ell = 0$ (dash-dotted line). For the first two cases, the curves cross the level 1 at $a_{\text{min}} \approx 0.84$ and $a_{\text{min}} \approx 2.44$, respectively. In turn, the third curve always remains greater than 1 (see explanations in Sec. 3.4). For $a = 0$, $\lambda_1$ is respectively equal to $2\pi^2$, $4\alpha^2$ and $5\pi^2$, where $\alpha \approx 2.4048$ is the first positive zero of the Bessel function $J_0(z)$.

3.2. Cross

Another example is a crossing of two perpendicular rectangular branches (Fig. 4a), for which the basic domain is again the unit square. Since the trial function (25) also satisfies the boundary condition for this problem, the previous sufficient condition (26) remains applicable for arbitrary lengths $a_3$ and $a_4$. This is not surprising because any increase of the basic domain (i.e., if the basic domain was considered as the unit square with two branches $Q_3$ and $Q_4$) decreases the eigenvalue. A symmetry argument implies that other consecutive pairs of branch lengths can be used in the condition (26), e.g., the eigenfunction is localized if $1/a_2 + 1/a_3 < 2$ for arbitrary $a_1$ and $a_4$. In turn, the condition $1/a_1 + 1/a_3 < 2$ is not sufficient for localization (in fact, taking $a_2 = a_4 = 0$ yields a rectangle without localization).

The specific feature of the cross is that the exterior boundary of the basic domain $\Omega$ consists of 4 corner points. We suggest another trial function

$$v(x, y) = x(1 + x) + y(1 + y), \quad (27)$$

which satisfies the Dirichlet boundary condition at these points. The direct integration yields

$$\beta = \frac{11}{90} \pi^2 - \frac{2}{3}, \quad \sigma_i = \frac{64}{\pi^6},$$

$$\kappa_i = 2\pi \sum_{n=2}^{\infty} \frac{1}{\sqrt{n^2 - 1}} \left( \frac{1 - (-1)^n}{\pi^3 n^3} \right)^2 \approx 0.0029.$$
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Figure 4. (a) Crossing of two rectangular branches; (b) an extension of the related basic domain $\Omega$; and (c) coupling between two waveguides from Fig. 2b ($\ell = 0$) with an opening of size $\varepsilon$.

The condition (14) reads now as
\[
\sum_{i=1}^{4} \frac{1}{a_i} < \frac{\beta}{\sigma_1} - \frac{\kappa_1}{\sigma_1} \sum_{i=1}^{4} \coth(\pi a_i \sqrt{3}).
\] (28)

If all the branches have the same length $a$, the upper bound of the minimal branch length can be estimated by solving the equation
\[
\frac{4}{a_{th}} = \frac{\beta}{\sigma_1} - \frac{4\kappa_1}{\sigma_1} \coth(\pi a_{th} \sqrt{3}),
\]
from which one gets $a_{th} \approx 0.2407$. Note that this result proves and further extends the prediction of localized eigenmodes in the crossing of infinite rectangular stripes which was made by Schult et al. by numerical computation [28]. In that reference, the importance of localized electron eigenstates in four terminal junctions of quantum wires was discussed.

Figure 5 presents first eigenfunctions for the crossing of two rectangular branches with $a_i = 5$ (the second eigenfunction, which looks similar to the third one, is not shown). As predicted by the sufficient condition (28), the first eigenfunction (with $\lambda_1 \approx 0.66\pi^2$) is clearly localized in the basic domain and exponentially decaying in the branches. In turn, all other eigenfunctions (with $\lambda_n > \pi^2$) are not localized.

It is worth noting again that any increase of the basic domain (see Fig. 4b) reduces the eigenvalue and thus favors the localization.

3.3. Bent strip

In previous examples, the basic domain was the unit square. We consider another shape for which the analytical estimates can be significantly advanced. This is a sector of the unit disk which can be seen as a connector between two parts of a bent strip (Fig. 2b). In contrast to the case of infinite stripes for which Goldstone and Jaffe have proved the existence of a localized eigenmode for any bending (except the straight strip) [12], there is a minimal branch length required for the existence of a localized eigenmode in a finite bent strip. In order to demonstrate this result, we consider the family of trial functions
\[
v_\alpha(r) = \frac{\sin \pi r}{r^\alpha} \quad (0 < \alpha < 1).
\] (29)
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$\lambda_1 \approx 0.661\pi^2$, $\lambda_2 = \lambda_3 \approx 1.032\pi^2$, $\lambda_4 \approx 1.036\pi^2$ and $\lambda_5 \approx 1.044\pi^2$.

Figure 5. First eigenfunctions for the crossing of two rectangular branches ($a_i = 5$). The associated eigenvalues are $\lambda_1 \approx 0.661\pi^2$, $\lambda_2 = \lambda_3 \approx 1.032\pi^2$, $\lambda_4 \approx 1.036\pi^2$ and $\lambda_5 \approx 1.044\pi^2$.

In Appendix B we derive Eqs. (B.1, B.2, B.3) for the coefficients $\beta$, $\sigma_i$, and $\kappa_i$, respectively. Since all these coefficients depend on $\alpha$, its variation can be used to maximize the threshold $\eta$ given by Eq. (24). The numerical computation of these coefficients suggests that $\eta$ is maximized for $\alpha$ around $1/3$: $\eta \approx 0.7154$. If $a_1 = a_2 = a$, one gets the upper bound $a_{th}$ of the minimal branch length which ensures the emergence of the localized eigenfunction:

$$a > a_{th} = \frac{2}{\eta} \approx 2.7956.$$  

We remind that this is sufficient, not necessary condition. The numerical computation of the first eigenvalue in the bent strip (by FEM implemented in Matlab PDEtools) yields $a_{min} \approx 2.44$. One can see that the upper bound $a_{th}$ is relatively close to this value. The behavior of the eigenvalue $\lambda_1$ as a function of the branch length $a$ is shown by dashed line on Fig. 3.

3.4. Waveguide without localization

Any increase of the basic domain $\Omega$ reduces the eigenvalues and thus preserves the localization. In turn, a decrease of $\Omega$ may suppress the trapped mode. For instance, the passage from L-shape ($\Omega$ being the unit square) to the bent strip ($\Omega$ being the quarter of the disk) led to larger minimal length required for keeping the localization ($a_{min} \approx 2.44$ instead of $a_{min} \approx 0.84$). For instance, when $a_1 = a_2 = 2$, the first eigenfunction, which was localized in the L-shape, is not localized in the bent strip (Fig. 6). Further decrease of the basic domain $\Omega$ may completely suppress the localization.

In order to illustrate this point, we consider the truncated L-shape shown on Fig. 2 with $\ell = 0$ for which

$$\Omega = \{(x, y) \in \mathbb{R}^2 : -1 < x < 0, -1 < y < 0, x + y > -1\}.$$
Figure 6. The first eigenfunction for three bent waveguides shown on Fig. 2 (ℓ = 0), with a = 2. The associate eigenvalue λ₁ is equal to 0.9357π², 1.0086π² and 1.1435π², respectively. Although the first eigenmode is localized, all three eigenfunctions visually look similar.

is a triangle. It is easy to see that $u(x, y) = \cos(\pi x) + \cos(\pi y)$ is the first eigenfunction of the following eigenvalue problem in $\Omega$:

$$-\Delta u = \tilde{\mu} u \quad \text{in} \ \Omega, \quad u|_\Gamma = 0, \quad \frac{\partial u}{\partial n}|_\Gamma = 0,$$

with the eigenvalue $\tilde{\mu}_1 = \pi^2$. From the variational principle

$$\tilde{\mu}_1 = \inf_{v \in H^1_0(\Omega), v \neq 0} \frac{(\nabla v, \nabla v)_{L^2(\Omega)}}{(v, v)_{L^2(\Omega)}},$$

so that

$$(\nabla v, \nabla v)_{L^2(\Omega)} \geq \tilde{\mu}_1 (v, v)_{L^2(\Omega)} = \pi^2 (v, v)_{L^2(\Omega)} \quad \forall v \in H^1_0(\Omega).$$

Moreover, the Friedrichs-Poincaré inequality in the branches $Q_i$ implies [22]

$$(\nabla v, \nabla v)_{L^2(Q_i)} \geq \pi^2 (v, v)_{L^2(Q_i)} \quad \forall v \in H^1_0(Q_i),$$

from which

$$(\nabla v, \nabla v)_{L^2(D)} \geq \pi^2 (v, v)_{L^2(D)} \quad \forall v \in H^1_0(D).$$

As a consequence, all eigenvalues of the original eigenvalue problem (11) in $D$ exceed $\pi^2$ and the corresponding eigenfunctions are not localized in the basic domain $\Omega$, whatever the length of the branches.

When one varies continuously $\ell$ in Fig. 2c, the basic domain transforms from the unit square (Fig. 2a) to triangle so that one can get any prescribed minimal length $a_{\min}$ between 0.84 and infinity. In other words, for any prescribed branch length, one can always design such a basic domain (such $\ell$) for which there is no localized eigenmodes. As a consequence, the localization may be very sensitive to the shape of the basic domain and to the length of branches. These effects which were overseen for infinite waveguides, may be important for microelectronic applications.

Figure 7 shows the first eigenfunction for three bent waveguides from Fig. 2 with $a = 20$. The associate eigenvalue $\lambda_1$ is equal to 0.9302π², 0.9879π² and 1.0032π², respectively. Although the last two values are very close to each other, the behavior of the associated eigenfunctions is completely different. According to the sufficient condition, the first two eigenfunctions are localized in the basic domain, while the last one is not. One can clearly distinguish these behaviors on Fig. 7.
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Figure 7. The first eigenfunction for three bent waveguides shown on Fig. 2 ($\ell = 0$), with $a = 20$. The associate eigenvalue $\lambda_1$ is equal to $0.9302\pi^2$, $0.9879\pi^2$ and $1.0032\pi^2$, respectively. Although the last two values are very close to each other, the behavior of the eigenfunctions is completely different.

3.5. Two coupled waveguides

The coupling of infinite waveguides has been intensively investigated [29]. We consider a coupling of two finite crossing waveguides through an opening of variable size $\varepsilon$ as shown on Fig. 4c. When $\varepsilon = 0$, one has two decoupled waveguides from Fig. 2c, for which we proved in the previous subsection the absence of localized eigenmodes. When $\varepsilon = \sqrt{2}$, there is no barrier and the waveguides are fully coupled. This is the case of crossing between two rectangular branches as shown on Fig. 4a, for which we checked the existence of localized eigenmodes under weak conditions (26) or (28). Varying the opening $\varepsilon$ from 0 to $\sqrt{2}$, one can continuously pass from one situation to the other. This transition is illustrated on Fig. 8 which presents the first eigenfunction for two coupled waveguides shown on Fig. 4c, with $a_i = 5$ and different coupling (opening $\varepsilon$). The first two eigenfunctions, with $\varepsilon = 0$ (fully separated waveguides) and $\varepsilon = 0.4\sqrt{2}$ (opening 40%), are not localized, while the last two eigenfunctions, with $\varepsilon = 0.5\sqrt{2}$ (opening 50%) and $\varepsilon = \sqrt{2}$ (fully coupled waveguides, i.e. a cross), are localized. The critical coupling $\varepsilon_c$, at which the transition occurs (i.e., for which $\lambda_1 = \pi^2$) lies between 40% and 50%. Although numerical computation may allow one to estimate $\varepsilon_c$ more accurately, we do not perform this analysis because the value $\varepsilon_c$ anyway depends on the branch lengths. In general, for any $a > a_{\text{min}} \approx 0.84$, there is a critical value $\varepsilon_c(a)$ for which $\lambda_1 = \pi^2$. For $\varepsilon < \varepsilon_c$, there is no localized modes, while for $\varepsilon > \varepsilon_c$ there is at least one localized mode. The high sensitivity of the localization character to the opening $\varepsilon$ and to the branch lengths can potentially be employed in quantum switching devices (see [30] and references therein).

Conclusion

We investigated the problem of trapped or localized eigenmodes of the Laplace operator in resonators with long branches that we called “finite waveguides”. In this context, the localization was understood as an exponential decay of an eigenfunction inside the branches. This behavior was related to the smallness of the associated eigenvalue $\lambda$ in comparison to the first eigenvalue of the Laplace operator in the cross-section of
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The first eigenfunction for two coupled waveguides shown on Fig. 4c, with $a_i = 5$ and different coupling (opening $\varepsilon$): $\varepsilon = 0$ (fully separated waveguides, zero coupling), $\varepsilon = 0.4\sqrt{2}$ (opening 40% of the diagonal), $\varepsilon = 0.5\sqrt{2}$ (opening 50% of the diagonal) and $\varepsilon = \sqrt{2}$ (fully coupled waveguides, no barrier). The associate eigenvalue $\lambda_1$ is equal to $1.05\pi^2$, $1.02\pi^2$, $0.97\pi^2$, and $0.67\pi^2$, respectively. In the first two cases, the eigenmodes is not localized. Changing the opening $\varepsilon$, one passes from non-localized to localized eigenmodes.

the branch with Dirichlet boundary condition. Using the explicit representation of an eigenfunction in branches, we proposed a general variational formalism for checking the existence of localized modes. The main result of the paper is the sufficient condition on the branch lengths for getting a trapped mode. In spite of the generality of the formalism, a practical use of the sufficient condition relies on an intuitive choice of the trial function in the basic domain (without branches). This function should be as close as possible to the (unknown) eigenfunction. Although there is no general recipe for choosing trial functions, one can often guess an appropriate choice, at least for relatively simple domains.

These points were illustrated for several typical waveguides, including 2D and 3D L-shapes, crossing of the rectangular stripes, and bent stripes. For all these cases, the basic domain was simple enough to guess an appropriate trial function in order to derive an explicit sufficient condition for getting at least one localized mode. In particular, we obtained the upper bound of the minimal branch length which is sufficient for localization. We proved the existence of a trapped mode in finite L-shape, bent strip and cross of two stripes provided that their branches are long enough, with an accurate estimate on the required minimal length. These results were confirmed by a direct numerical resolution of the original eigenvalue problem by finite element method implemented in Matlab PDEtools. The presented method can be applied for studying the localization in many other waveguides, e.g. smooth bent strip \[3\], sharply bent strip \[31\] or Z-shapes \[32\].

It is worth emphasizing that the distinction between localized and non-localized modes is much sharper in infinite waveguides than in finite ones. Although by definition the localized eigenfunction in a finite waveguide decays exponentially, the decay rate may be arbitrarily small. If the branch is not long enough, the localized mode may be visually indistinguishable from a non-localized one, as illustrated on Fig. \[6\]. In turn, the
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The main practical result is an explicit construction of two families of waveguides (truncated L-shapes on Fig. 2c and coupled waveguides on Fig. 4c), for which the minimal branch length $a_{\text{min}}$ for getting a trapped mode continuously depends on the parameter $\ell$ or $\varepsilon$ of the basic domain. For any prescribed (long enough) branch length, one can thus construct two almost identical finite waveguides, one with and the other without a trapped mode. The high sensitivity of the localization character to the shape of the basic domain and to the length of branches may potentially be used for switching devices in microelectronics.

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Appendix A. L-shape in three dimensions

As we mentioned at the end of Sec. 2, an extension to other types of branches is straightforward. We illustrate this point by considering the L-shape in three dimensions, i.e., two connected parallelepipeds of cross-section in the form of the unit square, for which the basic domain $\Omega$ is the unit cube (Fig. A1). For each branch, the eigenvalues and eigenfunctions in Eq. (18) for the cross-section can be parameterized by two indexes $m$ and $n$: $\nu_{m,n} = \pi^2(m^2 + n^2)$ and $\psi_{m,n}(y,z) = 2\sin(\pi my)\sin(\pi nz)$ (similar for the second branch).

We take the trial function

$$v(x,y,z) = [(1 + x)\sin(\pi y) + (1 + y)\sin(\pi x)]\sin(\pi z),$$

which satisfies the Dirichlet boundary condition. The coefficients $\beta$, $\sigma_i$ and $\kappa_i$ can be found from Eqs. (20, 21, 22), for which the explicit integration yields

$$(v,v)_{L_2(\Omega)} = \int_{-1}^{0} dx \int_{-1}^{0} dy \int_{-1}^{0} dz \ v^2 = \frac{1}{6} + \frac{1}{\pi^2},$$
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\[ (\nabla v, \nabla v)_{L^2(\Omega)} = \int_{-1}^{0} dx \int_{-1}^{0} dy \int_{-1}^{0} dz \left[ \left( \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial v}{\partial z} \right)^2 \right] = \frac{\pi^2}{3} + \frac{3}{2}, \]

so that \( \beta = 2\pi^2(\nabla v, \nabla v)_{L^2(\Omega)} - (v, v)_{L^2(\Omega)} = 1/2. \)

\[ (v, \psi_{1,1})_{L^2(\Gamma_1)} = \int_{-1}^{0} dy \int_{-1}^{0} dz \, v(0, y, z) \, 2 \sin(\pi y) \sin(\pi z) = \frac{1}{2}, \]

\[ (v, \psi_{m,n})_{L^2(\Gamma_1)} = \int_{-1}^{0} dy \int_{-1}^{0} dz \, v(0, y, z) \, 2 \sin(\pi my) \sin(\pi nz) = 0 \]

(for \( m \neq 1 \) or \( n \neq 1 \)), from which \( \sigma_1 = \sigma_2 = 1/4 \) and \( \kappa_1 = \kappa_2 = 0. \) The condition (19) reads as

\[ \frac{1}{a_1} + \frac{1}{a_2} < 2. \]

If the branches have the same length, \( a_1 = a_2 = a, \) then the upper bound of the minimal branch length for getting a localized eigenfunction is given by \( a_{th} = 1, \) as in two dimensions.

**Appendix B. Computation for bent strip**

The computation of the coefficients \( \beta \) and \( \sigma_i \) is straightforward, while that for \( \kappa_i \) requires supplementary estimates.

**Coefficient \( \beta. \)** One has

\[ (v, v)_{L^2(\Omega)} = \frac{\pi}{2} \int_{0}^{1} r^{1-2\alpha} \sin^2(\pi r) dr = \frac{\pi}{4} \left[ \frac{1}{2(1-\alpha)} - w_{2\alpha-1}(2\pi) \right], \]

where

\[ w_{\nu}(q) \equiv \int_{0}^{1} r^{-\nu} \cos(qr) dr. \]

Similarly,

\[ (\nabla v_\alpha, \nabla v_\alpha)_{L^2(\Omega)} = \frac{\pi^3}{2} \int_{0}^{1} r(v_\alpha')^2 dr = \frac{\pi}{2} \int_{0}^{1} r \left( \frac{\pi \cos \pi r}{r^\alpha} - \frac{\alpha \sin \pi r}{r^{1+\alpha}} \right)^2 dr. \]

Expanding the quadratic polynomial and integrating by parts, one gets

\[ (\nabla v_\alpha, \nabla v_\alpha)_{L^2(\Omega)} = \frac{\pi^3}{4} \left[ \frac{1}{2(1-\alpha)} + \frac{w_{2\alpha-1}(2\pi)}{1-2\alpha} \right]. \]

Combining this term with the previous result yields

\[ \beta = \frac{\pi^3}{4} \frac{2\alpha}{2\alpha - 1} w_{2\alpha-1}(2\pi). \quad (B.1) \]
In the limit $\alpha \to 1/2$, one has
\[
\lim_{\alpha \to 1/2} \frac{w_{2\alpha-1}(2\pi)}{2\alpha - 1} = \frac{\text{Si}(2\pi)}{2\pi} \approx 0.2257,
\]
where $\text{Si}(x)$ is the integral sine function.

**Coefficients** $\sigma_i$. For these coefficients, one gets

\[
(v, \sin(\pi r))_{L^2(\Gamma_1)} = \int_0^1 r^{-\alpha} \sin^2(\pi r)dr = \frac{1}{2} \left( \frac{1}{1 - \alpha} - w_\alpha(2\pi) \right),
\]
from which

\[
\sigma_1 = \sigma_2 = \frac{1}{2} \left( \frac{1}{1 - \alpha} - w_\alpha(2\pi) \right)^2. \tag{B.2}
\]

**Coefficients** $\kappa_i$. One considers

\[
(v, \sin(\pi nr))_{L^2(\Gamma_1)} = \int_0^1 r^{-\alpha} \sin(\pi r) \sin(\pi nr)dr
\]

\[
= \frac{1}{2} \left[ w_\alpha(\pi(n - 1)) - w_\alpha(\pi(n + 1)) \right].
\]

The function $w_\alpha(q)$ can be decomposed into two parts [33],

\[
w_\alpha(q) = \int_0^\infty r^{-\alpha} \cos(qr)dr - \int_1^\infty r^{-\alpha} \cos(qr)dr
= q^{\alpha-1} \sqrt{\frac{\pi}{2}} \frac{\Gamma(\frac{1-\alpha}{2})}{2^\alpha \Gamma(\frac{\alpha}{2})} - \tilde{w}_\alpha(q),
\]
where

\[
\tilde{w}_\alpha(q) \equiv \int_1^\infty r^{-\alpha} \cos(qr)dr.
\]

We have

\[
\kappa_i = 2\pi \sum_{n=2}^\infty \sqrt{n^2 - 1} \left( v, \sin(\pi nr) \right)_{L^2(\Gamma_1)}^2
= 2\pi \sum_{n=2}^\infty \sqrt{n^2 - 1} \left( d_n - e_n \right)^2,
\]
where

\[
d_n = \frac{\pi^{\alpha-\frac{1}{2}}}{2^{1+\alpha} \Gamma\left(\frac{\alpha}{2}\right)} \left[ (n - 1)^{\alpha-1} - (n + 1)^{\alpha-1} \right],
\]
\[
e_n = \frac{1}{2} \left[ \tilde{w}_\alpha(\pi(n - 1)) - \tilde{w}_\alpha(\pi(n + 1)) \right].
\]

In order to estimate the coefficients $e_n$, the function $\tilde{w}_\alpha(q)$ is integrated by parts that yields for $q = \pi(n \pm 1)$:

\[
\tilde{w}_\alpha(q) = \alpha \frac{\cos q}{q^2} - \alpha(\alpha + 1) \frac{\tilde{w}_{\alpha+2}(q)}{q^2}
= \alpha \frac{\cos q}{q^2} - \alpha(\alpha + 1)(\alpha + 2) \frac{\cos q}{q^4} + \alpha(\alpha + 1)(\alpha + 2)(\alpha + 3) \frac{\tilde{w}_{\alpha+4}(q)}{q^4}.
\]
The inequality
\[
(\alpha + 3)|\tilde{w}_{\alpha+4}(q)| \leq (\alpha + 3) \int_1^\infty r^{-\alpha-4} dr = 1
\]
leads to
\[
\alpha \frac{\cos q}{q^2} - \alpha(\alpha + 1)(\alpha + 2) \frac{\cos q + 1}{q^4} \leq \tilde{w}_\alpha(q) \leq \alpha \frac{\cos q}{q^2} - \alpha(\alpha + 1)(\alpha + 2) \frac{\cos q - 1}{q^4},
\]
from which
\[
e^-_n \leq e_n \leq e^+_n,
\]
where the lower and upper bounds are
\[
e^+_n = \frac{1}{2} \left[ \frac{\alpha}{\pi^2 (n+1)^2} - \frac{\alpha(\alpha + 1)(\alpha + 2) (1) \frac{\cos q + 1}{q^4}}{\pi^4 (n-1)^4} \right],
\]
Using these estimates, one gets
\[
\sum_{n=2}^{\infty} \sqrt{n^2 - 1} d_n^2 \equiv A_1,
\]
\[
\sum_{n=2}^{\infty} \sqrt{n^2 - 1} d_ne_n \geq \sum_{n=2}^{\infty} \sqrt{n^2 - 1} d_ne^-_n \equiv A^-_2,
\]
\[
\sum_{n=2}^{\infty} \sqrt{n^2 - 1} e^2_n \leq \sum_{n=2}^{\infty} \sqrt{n^2 - 1} (e^+_n)^2 \equiv A^+_3,
\]
from which
\[
\kappa_i \leq \kappa, \quad \kappa \equiv 2\pi (A_1 - 2A^-_2 + A^+_3).
\]
Although the expressions for \(A_1, A^-_2\) and \(A^+_3\) are cumbersome, the convergence of these series can be easily checked, while their numerical evaluation is straightforward.

The numerical computation of these coefficients shows that the threshold value \(\eta\) is maximized at \(\alpha \approx 1/3\): \(\eta \approx 0.7154\). Note that if the coefficients \(\kappa_i\) were computed by direct numerical integration and summation, the value of \(\eta\) for \(\alpha = 1/3\) could be slightly improved to be 0.7256. The difference results from the estimates we used, and its smallness indicates that the estimates are quite accurate.

[1] Duclos P and Exner P 1995 “Curvature-induced bound states in quantum waveguides in two and three dimensions” Rev. Math. Phys. 7 73-102
[2] Linton CM and McIver P 2007 “Embedded trapped modes in water waves and acoustics”, Wave Motion 45 16-29
[3] Olendski O and Mikhailovska L 2010 “Theory of a curved planar waveguide with Robin boundary conditions”, Phys. Rev. E 81 036606
[4] Rellich F 1948 Das Eigenwertproblem von in Halbrohren, (New York, Studies and Essays Presented to R. Courant) pp 329-344
[5] Jones DS 1953 “The eigenvalues of \(\nabla^2 u + \lambda u = 0\) when the boundary conditions are on semi-infinite domains”, Math. Proc. Camb. Phil. Soc. 49 668-684
Trapped modes in finite quantum waveguides

[6] Ursell F 1951 “Trapping modes in the theory of surface waves”, Math. Proc. Camb. Phil. Soc. 47 347-358
[7] Ursell F 1987 “Mathematical aspects of trapping modes in the theory of surface waves” J. Fluid Mech. 183 421-437
[8] Ursell F 1991 “Trapped Modes in a Circular Cylindrical Acoustic Waveguide”, Proc. R. Soc. Lond. A 435 575-589
[9] Parker R 1966 “Resonance effects in wake shedding from parallel plates: some experimental observations”, J. Sound Vib. 4 62-72
[10] Parker R 1967 “Resonance effects in wake shedding from parallel plates: calculation of resonance frequencies”, J. Sound Vib. 5 330-343
[11] Exner P and Seba P 1989 “Bound states in curved quantum waveguides”, J. Math. Phys. 30 2574-2580
[12] Goldstone J and Jaffe RL 1992 “Bound states in twisting tubes”, Phys. Rev. B 45 14100-14107
[13] Evans DV 1992 “Trapped acoustic modes”, IMA J. Appl. Math. 49 45-60
[14] Evans DV, Levitin M and Vassiliev D 1994 “Existence theorems for trapped modes”, J. Fluid Mech. 261 21-31
[15] Davies EB and Parnovski L 1998 “Trapped modes in acoustic waveguides”, Q. J. Mech. Appl. Math. 51 477-492
[16] Bulla W, Gesztesy F, Renger W and Simon B 1997 “Weakly coupled bound states in quantum waveguides”, Proc. Amer. Math. Soc. 125 1487-1495
[17] Bonnet-Ben Dhia AS and Joly P 1993 “Mathematical analysis of guided water waves”, SIAM J. Appl. Math. 53 1507-1550
[18] Sapoval B, Gobron T and Margolina A 1991 “Vibrations of fractal drums”, Phys. Rev. Lett. 67 2974
[19] Even C, Russ S, Repain V, Pieranski P and Sapoval B 1999 “Localizations in Fractal Drums: An Experimental Study”, Phys. Rev. Lett. 83 726
[20] Felix S, Asch M, Filoche M and Sapoval B 2007 “Localization and increased damping in irregular acoustic cavities”, J. Sound. Vibr. 299 965
[21] Jackson JD 1999 Classical Electrodynamics, 3rd Ed. (New York: Wiley & Sons)
[22] Lions JL and Magenes E 1972 Non-homogeneous boundary value problems and applications (Berlin, New York: Springer-Verlag)
[23] Birman MS 1961 “O spektrre singulyarnix granichnix zadach” Math. Sb. 55 125-174 [in Russian].
[24] Schwinger J 1961 “On the bound states of a given potential” Proc. Nat. Acad. Sci. 47 122-129.
[25] Aslany’an AG, Vasil’ev DG and Lidskii VB 1981 “Frequencies of free vibrations of a thin shell interacting with a liquid” Funkt. Anal. Appl. 15 157-164
[26] Levitin M and Marletta M 2008 “A simple method of calculating eigenvalues and resonances in domains with infinite regular ends” Proc. Royal Soc. Edinburgh 138A 1043-1065
[27] Delitsyn AL 2004 “The Discrete Spectrum of the Laplace Operator in a Cylinder with Locally Perturbed Boundary”, Diff. Eq. 40 207-217
[28] Schult RL, Ravenhall DG and Wyld HW 1989 “Quantum bound states in a classically unbound system of crossed wires”, Phys. Rev. B 39 5476-5479
[29] Exner P, Seba P, Tater M and Vanek D 1996 “Bound states and scattering in quantum waveguides coupled laterally through a boundary window”, J. Math. Phys. 37 4867
[30] Timp G, Baranger HU, deVegvar P, Cunningham JE, Howard RE, Behringer R and Mankiewich PM 1988 “Propagation around a Bend in a Multichannel Electron Waveguide”, Phys. Rev. Lett. 60 2081-2084
[31] Carini JP, Londergan JT, Mullen K and Murdock DP 1993 “Multiple bound states in sharply bent waveguides”, Phys. Rev. B 48 4503-4515
[32] Carini JP, Londergan JT, Murdock DP, Trinkle D and Yung CS 1997 “Bound states in waveguides and bent quantum wires. I. Applications to waveguide systems”, Phys. Rev. B 55 9842
[33] Gradsteyn IS and Ryzhik IM 1980 Table of Integrals, Series and Products (New York: Academic
Trapped modes in finite quantum waveguides

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