Localization of Neumann eigenfunctions near irregular boundaries

Peter W Jones and Stefan Steinerberger

Department of Mathematics, Yale University, New Haven, CT 06511, United States of America
E-mail: jones@math.yale.edu and stefan.steinerberger@yale.edu

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Abstract
It has been empirically observed that eigenfunctions of Laplace’s equation \(-\Delta \phi = \lambda \phi\) with Neumann boundary conditions sometimes localize near the boundary of the domain if that boundary is rough (say, fractal). This has some nontrivial implications in acoustics that has been put to real-life use (sound attenuation by noise-protective walls); this short paper describes the mathematical mechanism responsible for this and describes the quantitative strength of the phenomenon for some examples.

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1. Introduction

1.1. Introduction

This short paper is concerned with an interesting localization phenomenon that has been observed to occur for eigenfunctions of the Laplace operator with Neumann boundary conditions. Let us fix an open, bounded domain \(\Omega \subset \mathbb{R}^n\) (our subsequent argument also works on manifolds and, with some modifications, on finite graphs) and consider

\[-\Delta u = \mu u \quad \text{inside } \Omega\]
\[\frac{\partial u}{\partial \eta} = 0 \quad \text{on } \partial \Omega.

It is known that there is a discrete sequence of eigenvalues \(0 = \mu_0 < \mu_1 \leq \mu_2 \leq \ldots\) for which there is a solution and we will refer to these solutions as the eigenfunctions of the Neumann

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Laplacian. These solutions can only be realized as critical points of the Rayleigh–Ritz energy functional and

\[ u_k = \arg \min_{u \in V_{k-1}} \frac{\int_\Omega |\nabla u|^2 \, dx}{\int_\Omega u^2 \, dx}, \]

where \( V_{k-1} = \text{span} \{ u_1, \ldots, u_{k-1} \} \) (this statement is also known as the Courant–Fischer–Weyl Minimax theorem). This formulation shows that we need only minimal assumptions on the domain \( \Omega \), in particular, this formulation is perfectly reasonable on fractal domains \([17,18,22]\). On fractal domains, the computation of these functions comes with new numerical challenges that are interesting in their own right \([4,19,23]\). Moreover, the variational formulation also easily translates to combinatorial graphs; the arising spectral theory has had tremendous applications in computer science \([8]\). Even on simple smooth domains, the localization behavior of these eigenfunctions is an important fundamental concept which we do not summarize here (see \([1–3,12–14,24,32]\) and references for examples of classical and recent work on this).

1.2. Cheeger-type inequalities

It is well understood that if \( \Omega \) is comprised of essentially two domains connected by a thin connecting set, then the first Neumann eigenfunction is approximately constant in each cluster (the gradient is localized in the thin connection); this is valuable in applications \([8,9]\) where it allows for a spectral approach to partitioning a set into two parts in a ‘natural’ way.

An example is given in figure 1: the first nontrivial Neumann eigenfunction will be essentially constant on each side of the dumbbell manifold and smoothly transition in the ‘bridge’ (thus concentrating the gradient on a set of small measure). These kinds of phenomena have been made precise in classical works of Cheeger \([7]\), Buser \([6]\) and many others. There is continuous ongoing work because of the profound relevance in computer science (see e.g. \([20]\)).

1.3. A specific localization phenomenon

We focus on a very different and somewhat more subtle phenomenon that has been actively studied by Sapoval, collaborators and others \([10,11,15,16,24–30]\).

A suitable example, taken from Felix et al \([10]\), is shown in figure 2: for these two domains, one can numerically observe the existence of localized Neumann eigenfunctions that are localized close to the irregular boundary (in the ‘spikes’ and between the slit, respectively). Moreover, these eigenfunctions are not exotic high-frequency objects but correspond to small low-lying eigenvalues (the examples given in the survey of Grebenkov and Nguyen \([14]\) exhibit that phenomenon for the 10th and the 12th eigenfunction). It can also be numerically
observed that the strength of the localization phenomenon depends on the width of the slits and the angles of the cones, respectively. Narrower slits and smaller angle for cones lead to a stronger degree of localization. We refer to the survey of Grebenkov and Nguyen [14, section 7.6.] for a more detailed discussion of the phenomenon. As is observed in [10], the presence of irregular boundaries seems to cause some of the Neumann eigenfunctions to localize there even though these irregularities do not necessarily separate a subdomain from the rest of the domain in any obvious way (this is what strongly differentiates the phenomenon from other localization phenomena).

1.4. Application in acoustics

This has some nontrivial implications in acoustics. The Neumann boundary condition represents the physical boundary condition for acoustic waves velocity (the gradient of acoustic pressure) on a rigid boundary—as a consequence, the phenomenon of localization occurs in practice and has even been used in the construction of road noise barriers ([10] refers to the Fractal Wall™, product of Colas Inc., French patent No. 0203404). What complicates matters, again referring to the domain shown in figure 2, is that the localization is not as pronounced as in classical examples in mathematical physics where a localized eigenfunction undergoes exponential decay away from the area where it is localized. Here, there is no exponential decay in the rest of the domain—moreover, the localized eigenfunctions on the domain with spikes do not necessarily localize within a single ‘spike’ but in several neighboring spikes at the same time.

1.5. The origin of the phenomenon

The cause of the phenomenon has been mysterious for a while: originally it was believed to be a phenomenon mainly found in fractal domains. A 2010 Notices articles of Heilman and Strichartz [16] gives non-fractal examples and instead puts an emphasis on the role of symmetries; the recent survey of Grebenkov and Nguyen [14] remarks ‘symmetry is neither sufficient nor necessary for localization’. One of the main contributions of our paper is to explain the origin of the phenomenon and show that it neither requires a fractal domain nor does it depend on symmetries: it is a function of concentration of the heat kernel or, phrased differently, a function of Brownian motion particles being trapped (something that is easier to accomplish in fractal domains). Heilman and Strichartz also remark that ‘We do not have to go very high up in the spectrum’ (to find these localized eigenfunctions); this observation is also confirmed by our explanation.
2. A proof of localization

2.1. Idea

There is a fairly simple explanation for the phenomenon: the irregular boundary ‘traps’ Brownian motion (which is reflected) for an extended period of time and this leads to the creation of localized eigenfunctions. Put differently, and this is how we will phrase our derivation that avoids the notion of Brownian motion altogether, the heat kernel is more strongly localized than it would be in free space.

We will now explain the underlying idea (see figure 3) and apply it to the two domains in figure 2. It is not hard to use the idea to derive explicit statements in various other settings. Let \( p(t,x,y) \) denote the Neumann heat kernel

\[
p(t,x,y) = \sum_{k=0}^{\infty} e^{-\mu_k t} \phi_k(x) \phi_k(y).
\]

We recall that \( p(t,x,y) \geq 0 \), that for all \( x \in \Omega \) and all \( t > 0 \)

\[
\int_{\Omega} p(t,x,y) dy = 1
\]

and that \( p(t,x,y) = p(t,y,x) \). In free Euclidean space, \( p(t,x,\cdot) \) is merely a Gaussian centered at \( x \) and localized at spatial scale \( \sim \sqrt{t} \). The probabilistic interpretation is that of \( p(t,x,\cdot) \) as describing the distribution of a Brownian motion particle started at \( x \), running for time \( t > 0 \) and being reflected upon impact on the boundary. For very irregular boundaries, there might be some difficulty in defining the notion of a reflected Brownian motion, however, we only work in settings where Neumann eigenfunctions of the Laplacian are defined.

The key identity that underlies the phenomenon is

\[
\int_{\Omega} p(t,x,y)^2 dy = \int_{\Omega} \left( \sum_{k=0}^{\infty} e^{-\mu_k t} \phi_k(x) \phi_k(y) \right)^2 dy
\]

\[
= \int_{\Omega} \sum_{k,\ell=0}^{\infty} e^{-\mu_k t} e^{-\mu_\ell t} \phi_k(x) \phi_k(y) \phi_\ell(x) \phi_\ell(y) dy
\]

\[
= \sum_{k=0}^{\infty} e^{-2\mu_k t} \phi_k(x)^2.
\]

This identity can be used in both directions: if \( p(t,x,\cdot) \) is strongly concentrated around \( x \) (which happens if the boundary \( \partial \Omega \) has a trapping effect on Brownian motion), then this implies that at least some of the Neumann eigenfunctions have to be large in \( x \). Moreover, these eigenfunctions have to correspond to a relatively small eigenvalue, large values arising for large eigenvalues are dampened the exponential decay and play no role. Conversely, if \( p(t,x,\cdot) \) is spread out, then none of the low-frequency eigenfunctions can be concentrated in \( x \) beyond a certain degree. The parameter \( t > 0 \) is arbitrary and has the effect of fixing a natural length scale \( \sim \sqrt{t} \) and an associated frequency range of eigenvalues that play a role.

3. Scaling and some examples

The purpose of this Section is to point out the natural scales of these objects in the case of \( \Omega \subset \mathbb{R}^2 \) since all the examples in this paper are 2D. However, we hasten to emphasize that
the higher-dimensional case (or the manifold setting) can be dealt with in exactly the same way. Ignoring (small) contributions from possibly fractal boundaries (see [5, 17]), we expect $\mu_k \sim c k$ on 2D domains with an implicit constant $c > 0$ depending only on the measure $|\Omega|$ of the domain. We also observe that in the case of all eigenfunctions being relatively flat, i.e. $\phi_k(x)^2 \sim 1$, we expect

$$
\sum_{k=1}^{\infty} e^{-\mu_k t} \phi_k(x)^2 \sim \sum_{k=1}^{\infty} e^{-\mu_k t} \sim \sum_{k=1}^{\infty} e^{-ckt} = \frac{1}{e^t - 1} \sim \frac{1}{ct}.
$$

Naturally, this chain of equivalences can be made in a variety of possible ways under a variety of different assumptions. We will now compute the left-hand side for domains $\Omega \subset \mathbb{R}^2$ that behave like the figure on the left-hand side of figure 2 (a square with thin cones attached). We first compute it for points $x$ inside $\Omega$ that are far away from the boundary $d(x, \partial \Omega) \gtrsim \sqrt{t}$. Points far away from the boundary have a short-time heat kernel asymptotic dictated by Varadhan’s Lemma [33]. This suggests, in two dimensions, that

$$
p(t,x,y) \sim \frac{1}{(4\pi t)^2} e^{-\frac{|x-y|^2}{4t}}
$$

and thus

$$
\int_{\Omega} p(t,x,y)^2 dy \sim \frac{1}{8\pi t}.
$$

This is very much in correspondence with what we would expect under the assumption that $\phi_k(x)^2 \sim 1$ for all $k$. However, the situation inside a cone is different.

We use the reflection trick to compute the integral for $x$ at distance $\backsimeq \sqrt{t}$ from the apex of a cone with opening angle $\alpha$ and sides of length at least $\sim \sqrt{t}$ (see figure 4). We obtain, in order of magnitude,

$$
\int_{\Omega} p(t,x,y)^2 dy \sim \frac{2\pi}{\alpha} \frac{1}{8\pi t} = \frac{1}{\alpha 4t}.
$$

This, however, is much larger than the corresponding quantity in free-space if $\alpha$ is small and implies

$$
\sum_{k=0}^{\infty} e^{-2\mu_k t} \phi_k(x)^2 \sim \frac{1}{\alpha 4t}
$$

which forces some of the low-lying eigenfunctions to be large in $x$. We observe that this does not imply exponential localization (which would be false) nor does it imply that there is an eigenfunction that is large close to the apex of exactly one cone (which would also be false): it only implies that there exists an eigenfunction for which $e^{-\mu_k t} \phi_k(x)^2 \gtrsim \alpha^{-1} t^{-1}$ which is a factor of $\sim \alpha^{-1}$ larger than one would expect for a function at scale $\sim 1$. This is only possible for $\mu_k$ small and thus also explains why these localized objects are observed at rather low frequencies.

3.1. Another example: the slit

We illustrate this fundamental principle in a second case: that of a slit introduced in a 2D domain $\Omega$ (see figure 2). Let us assume, for simplicity, that the slits are of size $\sim 1 \times 0.01$ each and that they are distance $\delta$ apart from each other (the constant 0.01 is somewhat arbitrary and chosen for illustrative purposes, it could of course be arbitrarily small). Let us pick $x$ to be the point in the center between the two slits and let us fix $t = 1$. We observe that the likelihood of Brownian motion escaping the regions $R$ between these two slits, a region of area $\sim \delta$, is bounded away from 0 (see figure 5).

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This means that
\[ 1 \lesssim \int_R p(1,x,y)dy \leq \delta^{1/2} \left( \int_R p(1,x,y)^2dy \right)^{\frac{1}{2}} \]
and thus
\[ \sum_{k=0}^{\infty} e^{-2\mu_k} \phi_k(x)^2 \gtrsim \frac{1}{\delta}. \]
This determines the scale at which the localization phenomenon increases as the two slits move closer to each other. All of this can be made precise under some assumption on the domain \( \Omega \) (which determines the scaling of \( \mu_k \)).

3.2. Non-localization

There is also a converse implication whenever a point \( x \) is far from the boundary, thus allowing for an unobstructed diffusion of the Green’s function and implies that
\[ \int_{\Omega} p(t,x,y)^2dy \sim \frac{1}{t} \]
will behave as in free space.

In that case, none of the first few eigenfunctions can be very large in \( x \) (unless many more vanish which would imply them localizing somewhere else). This has an interesting implication for domains such as the ones displayed in figure 2: the boundary is actually piecewise-linear comprised of finitely many pieces. This shows that the only point in which diffusion can truly be trapped in the sense above, is close to the apex of a cone for the domain shown on the left in figure 2. Moreover, diffusion cannot be trapped at all in the slit domain as soon as \( t \lesssim \delta^2 \).

For the domain with a slit this reasoning suggests, under some control on the eigenvalues and assuming an otherwise smooth boundary \( \partial \Omega \), that above a certain frequency no eigenfunction will be particularly localized. Conversely, in the presence of cone structures the argument suggests the existence of infinitely many eigenfunctions that have substantial size close to the apex.

3.3. Another example: fractals

Returning to the original question of the behavior of eigenfunctions near the boundary of irregular or possibly even fractal domains, we see that the main question is whether diffusion gets trapped or whether it spreads freely. It is natural to ask whether the speed of diffusion (and thus, by the argument above, the strength of the localization of Neumann eigenfunctions) is somehow related to the Hausdorff dimension (or maybe the Minkowski dimension, see Lapidus [17, 18]) of the fractal.

We consider one explicit example for the sake of clarification by taking a sequence of disks of radius \( r_n = 2^{-n} \) that are glued together along line segments of length \( 2^{-4n} \) (see figure 6).

**Proposition.** Some eigenfunctions exhibit exponential growth in the balls.

We observe that the same result is true for eigenfunctions of the Dirichlet Laplacian for rather trivial reasons: the narrow connection between two adjacent balls essentially separates these domains completely, eigenfunctions localize and thus scale with the inverse volume that decays exponentially—hence exponential growth. Eigenfunctions of the Neumann–Laplacian behave differently, there is no reason why they would be small in a slit connecting two balls.
Proof. The argument is a slight modification of the previous arguments (but still relying on the same mechanism). Pick $\chi_n$ to be the characteristic function of the $n$th ball. We apply the Neumann heat equation for time $t = 1$ and obtain

$$e^{\Delta t} \chi_n = \sum_{k=0}^{\infty} e^{-\mu k} \langle \chi_n, \phi_k \rangle \phi_k.$$ 

It follows from known estimates on the narrow escape problem [31] that for this choice of parameters $e^{\Delta t} \chi_n \geq \chi_n / 2$. The Cauchy–Schwarz inequality implies
\[ |\langle \chi_n, \phi_k \rangle| \leq \| \chi_n \|_{L^2} \| \phi_k \|_{L^2} = \| \chi_n \|_{L^2} \leq c \cdot 2^{-n}. \]

Altogether, plugging in a point \( x \) from the \( n \)th ball, we obtain
\[ \frac{1}{2} \leq e^{\Delta} \chi_n(x) = \sum_{k=0}^{\infty} e^{-\mu_k} \langle \chi_n, \phi_k \rangle \phi_k \leq c \cdot 2^{-n} \sum_{k=0}^{\infty} e^{-\mu_k} |\phi_k(x)|. \]

This shows
\[ \sum_{k=0}^{\infty} e^{-\mu_k} |\phi_k(x)| \geq 2^{n-1}/c \quad \text{for } x \text{ in the } n \text{th ball}. \]

3.4. Related results

The entire approach is in a similar spirit as work of the second author [32] giving an interpretation of localization properties in terms of diffusion. Moreover, the same functional has recently been used by J. Lu and the second author [21] where a discrete heat kernel was used to determine the location of localized eigenvectors associated to linear system \( Ax = \lambda x \). In particular,
\[ \int_{\Omega} p(t, x, y)^2 \, dy \text{ can be used to detect localized eigenfunctions.} \]

The paper [21] also discusses fast linear algebra methods for its computation.

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ORCID iDs

Stefan Steinerberger  https://orcid.org/0000-0002-7745-4217

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