# Estimates on Neumann eigenfunctions at the boundary, and the “Method of Particular Solutions" for computing them

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# Outline

# Introduction

The Method of Particular Solutions is a numerical method for finding eigenvalues and eigenfunctions of the Laplacian on a Euclidean domain.

- We choose an energy $E > 0$, and then look for a solution to the Helmholtz equation $(\Delta - E)u = 0$ that approximately satisfies the boundary condition.
- We look for estimates telling us how close $E$ is to the spectrum, in terms of the boundary condition error.
- Want estimates that are sharp for $E \to \infty$.

Dirichlet BC: Barnett, Barnett-Hassell arXiv:1006.3592v1.
Neumann BC: Barnett-Hassell (in progress).

In this section I will consider the Dirichlet Laplacian $\Delta$ on a smooth, bounded domain $\Omega$ in $\mathbb{R}^n$. As is well known, $\Delta$ is self-adjoint on the domain $H^2(\Omega) \cap H_0^1(\Omega)$, and has an orthonormal basis of real eigenfunctions $u_j \in L^2(\Omega)$ with eigenvalues $E_j = \lambda_j^2$ of finite multiplicity:

$$0 < \lambda_1 < \lambda_2 \leq \cdots \to \infty.$$

By definition, the Dirichlet eigenfunctions $u_j$ vanish when restricted to the boundary. Let $\psi_j$ denote the normal derivative of $u_j$ at the boundary, taken with respect to the exterior unit normal $n$:

$$\psi_j = d_n u_j \big|_{\partial\Omega} \in C^\infty(\Omega).$$

Let's prove that there are upper and lower bounds

$$C^{-1}\lambda_j \le \|\psi_j\|_{L^2(\partial\Omega)} \le C\lambda_j \tag{1}$$

where $C$ depends only on $\Omega$. These are easily proved using Rellich-type identities, involving the commutator of $\Delta$ with a suitably chosen vector field $V$. The basic computation is

$$\langle u, [\Delta, V]u\rangle = \int_\Omega \Big(((\Delta - \lambda^2)u)(Vu) - u(V(\Delta - \lambda^2)u)\Big) + \int_{\partial\Omega} \Big((d_n u)(Vu) - u(d_n(Vu))\Big). \tag{2}$$

If $u = u_j$ is a Dirichlet eigenfunction with eigenvalue $\lambda_j^2$, then three of the terms on the RHS vanish, and we obtain

$$\langle u, [\Delta, V]u\rangle = \int_{\partial\Omega} (d_n u)(Vu).$$

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If we choose $V$ equal to the exterior unit normal then the RHS is precisely $\|\psi_j\|^2$. The left hand side is $\langle u, Qu\rangle$ where $Q$ is a second order differential operator and is $O(\lambda_j^2)$, yielding the upper bound $\|\psi_j\|^2 = O(\lambda_j^2)$.

On the other hand, if we take $V$ to be the vector field $\sum_i x_i \partial_{x_i}$, then $[\Delta, V] = 2\Delta$. Then the LHS is exactly equal to $2\lambda_j^2$, while the RHS is no bigger than $(\max_{\partial\Omega} |x|)\|\psi_j\|^2$, yielding the lower bound $\lambda_j^2 = O(\|\psi_j\|^2)$.

It turns out that there is a very useful generalization of the upper bound in (1), proved recently by Barnett and the speaker, that applies to a whole $O(1)$ frequency window:

**Theorem**

*Let $\Omega \subset \mathbb{R}^n$ be a smooth bounded domain and let $\psi_i$ be defined as above. Then the operator norm of*

$$\sum_{\lambda_i \in [\lambda, \lambda+1]} \psi_i \langle \psi_i, \cdot \rangle \quad : L^2(\partial\Omega) \to L^2(\partial\Omega) \tag{3}$$

*is bounded by $C\lambda^2$, where $C$ depends only on $\Omega$.*

- This is quite a strong estimate, since there is a lower bound of the form $c\lambda^2$ on the operator norm of any *one* term in the sum.
- This is closely related to the phenomenon of 'quasi-orthogonality' of $\psi_i$ and $\psi_j$, when $|\lambda_i - \lambda_j|$ is small. Indeed, this estimate implies that when $|\lambda_i - \lambda_j| \leq 1$, then the inner product $\langle \psi_i, \psi_j \rangle$ is usually small compared with $\lambda^2$.
- It is closely related to an identity of Bäcker, Fürstberger, Schubert and Steiner (2002).

Theorem 1 is proved as follows: first, we prove the upper bound $\|d_n u\|_{L^2(\partial\Omega)} \leq C\lambda\|u\|_{L^2(\Omega)}$ is valid not just for eigenfunctions, but for approximate eigenfunctions $u \in \operatorname{dom}\Delta$ such that

$$\|(\Delta - \lambda^2)u\|_{L^2(\Omega)} = O(\lambda).$$

In fact, the proof is almost unchanged; see (2); also Xu. Notice that this condition applies in particular to a spectral cluster, that is, for $u \in \operatorname{range} E_{[\lambda,\lambda+1]}(\sqrt{\Delta})$. We then use a $TT^*$ argument:

We define an operator $T$ from range $E_{[\lambda,\lambda+1]}(\sqrt{\Delta})$ to $L^2(\partial\Omega)$ by $Tu = d_n u|_{\partial\Omega}$. That is,

$$Tu = \sum_{\lambda_i \in [\lambda,\lambda+1]} \langle u, u_i \rangle \psi_i .$$

Then we have, by the previous page,

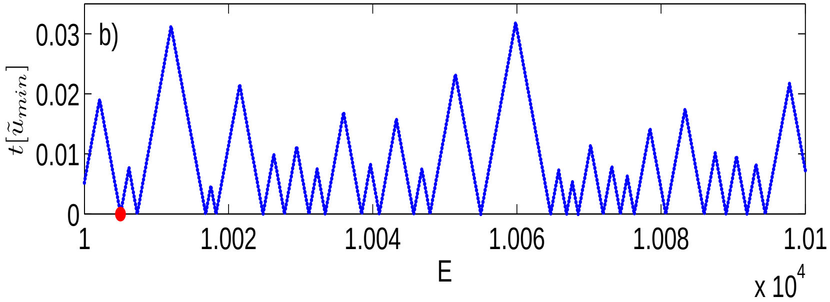
$$\|T\| \leq C\lambda.$$

It follows that $TT^* : L^2(\partial\Omega) \to L^2(\partial\Omega)$ has operator norm bounded by $C^2\lambda^2$. But $TT^*$ is precisely the operator (3) appearing in the statement of the theorem.

In the method of particular solutions (MPS), one chooses an energy $E = \lambda^2$ and then tries numerically to minimize the quantity

$$t[u] = \frac{\|u\|_{L^2(\partial\Omega)}}{\|u\|_{L^2(\Omega)}} \tag{4}$$

over all nontrivial solutions of $(\Delta - \lambda^2)u = 0$. Clearly, if $t[u] = 0$, then $u$ is a Dirichlet eigenfunction. But this cannot happen unless $\lambda^2$ happens to be an exact Dirichlet eigenvalue, so generally we can only hope to minimize $t[u]$, or more precisely to find a $u$ for which $t[u]$ is close to $\inf t$.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**Question:** If $t[u]$ is small, can we say quantitatively that $\lambda^2$ is close to a Dirichlet eigenvalue?
An answer to this question is provided by the Moler-Payne inclusion bound. This says that

$$d(\lambda^2, \mathrm{spec}_D) \leq C\lambda^2 t[u],$$

where $C$ depends only on $\Omega$. The proof uses very little about the Dirichlet problem in particular.

Recently, Alex Barnett, and then Barnett and myself, improved this bound by a factor of $\lambda$:

## Theorem

*There exist constants* $c, C$ *depending only on* $\Omega$ *such that the following holds. Let* $u$ *be a nonzero solution of* $(\Delta - \lambda^2)u = 0$ *in* $C^\infty(\Omega)$*. Let* $t[u] = \|u|_{\partial\Omega}\|_{L^2(\partial\Omega)} / \|u\|_{L^2(\Omega)}$*, and let* $u_{\min}$ *be the Helmholtz solution minimizing* $t[u]$*. Then*

$$c\lambda t[u_{\min}] \leq d(\lambda^2, \mathrm{spec}_D) \leq C\lambda t[u].$$

**Proof:** The result is trivial if $\lambda^2 \in \mathrm{spec}_D \Delta$. Suppose that $\lambda^2$ is not an eigenvalue, and consider the map $Z(\lambda)$ that takes $f \in L^2(\partial\Omega)$ to the solution $u$ of the equation

$$(\Delta - \lambda^2)u = 0, u|_{\partial\Omega} = f.$$

The $u$ that minimizes $t[u]$ then maximizes $\|u\|_{L^2(\Omega)}$ given $\|u\|_{L^2(\partial\Omega)}$. So

$$(\min t[u])^{-1} = \|Z(\lambda)\| \implies (\min t[u])^{-2} = \|A(\lambda)\|,$$

where the operator $A(\lambda) := Z(\lambda)^* Z(\lambda) : L^2(\partial\Omega) \to L^2(\partial\Omega)$ has the expression (Barnett)

$$A(\lambda) = \sum_j \frac{\psi_j \langle \psi_j, \cdot \rangle}{(\lambda^2 - \lambda_j^2)^2}. \tag{5}$$

(strop) To prove (5), we show that $Z(\lambda)$ has the expression

$$Z(\lambda)f = \sum_i \frac{\langle f, \psi_i \rangle u_i}{\lambda^2 - \lambda_i^2} \tag{6}$$

from which (5) follows immediately. To express $Z(\lambda)$, suppose $f$ is given and $u = Z(\lambda)f$. We write $u = \sum a_i u_i$ as a linear combination of Dirichlet eigenfunctions. Then

$$a_i = \langle u, u_i \rangle = \frac{1}{\lambda^2 - \lambda_i^2} \int_\Omega \big( (\Delta u) u_i - u(\Delta u_i) \big)$$

$$= \frac{1}{\lambda^2 - \lambda_i^2} \int_{\partial\Omega} \big( u(d_n u_i) - (d_n u) u_i \big) = \frac{1}{\lambda^2 - \lambda_i^2} \int_{\partial\Omega} f \psi_i$$

which proves (6).

The lower bound in Theorem 2 is easy to prove: we note that $A(\lambda)$ is a sum of positive operators in (5), so the operator norm of $A(\lambda)$ is bounded below by the operator norm

$$\|A(\lambda)\| \geq \Big\| \frac{\psi_j \langle \psi_j, \cdot \rangle}{(\lambda^2 - \lambda_j^2)^2} \Big\| \geq \frac{c\lambda^2}{d(\lambda^2, \mathrm{spec}_D)^2},$$

where $\lambda_j$ is the closest eigenfrequency to $\lambda$. Since $(\min t[u])^{-2} = \|A(\lambda)\|$, this proves the lower bound.

To prove the upper bound, we use Theorem 1. We need to show that

$$\|A(\lambda)\| \leq \frac{C\lambda^2}{d(\lambda^2, \mathrm{spec}_D)^2}. \tag{7}$$

To show that $\|A(\lambda)\| \leq C\lambda^2 d(\lambda^2, \mathrm{spec}_D)^{-2}$, we break up the sum (5) into the 'close' eigenfrequencies in the interval $[\lambda - 1, \lambda + 1]$ and the rest. The estimate above for the close eigenvalues is immediate from Theorem 1. The far eigenvalues are estimated using Theorem 1 together with exploiting the denominator $(\lambda^2 - \lambda_j^2)^2$, and make a smaller contribution.

We want to consider the MPS for computing Neumann eigenvalues and eigenfunctions. The Neumann boundary condition is $d_n u|_{\partial\Omega} = 0$. It seems logical to minimize (cf. (4))

$$t_{\mathrm{Id}}[u] = \frac{\|d_n u\|_{L^2(\partial\Omega)}}{\|u\|_{L^2(\Omega)}},$$

over nontrivial solutions $u$ of $(\Delta - E)u = 0$, since $t_{\mathrm{Id}}[u] = 0$ implies that $E$ is a Neumann eigenvalue and $u$ a Neumann eigenfunction. We could equally well minimize the quantity

$$t_F[u] = \frac{\|F(d_n u)\|_{L^2(\partial\Omega)}}{\|u\|_{L^2(\Omega)}},$$

for any invertible operator $F$ on $L^2(\partial\Omega)$. It turns out that there is an essentially optimal choice of $F$, which is **not** the identity.

The form of $F$ is suggested by the local Weyl law for boundary values of eigenfunctions. This law (Gérard-Leichtnam, H.-Zelditch) says that the boundary values of eigenfunctions are distributed in phase space $T^*(\partial\Omega)$ (in the sense of expectation values $h_j^2\langle\psi_j, A_{h_j}\psi_j\rangle$ or $\langle w_j, A_{h_j} w_j\rangle$) according to

$$\begin{gathered} c(1-|\eta|^2)^{1/2} 1_{\{|\eta|\leq 1\}} \text{ (Dirichlet)}, \\ c(1-|\eta|^2)^{-1/2} 1_{\{|\eta|\leq 1\}} \text{ (Neumann)}. \end{gathered} \tag{8}$$

Here $\eta \in T^*(\partial\Omega)$ and we adopt the semiclassical scaling, that is the frequencies at eigenvalue $\lambda_j^2$ are scaled by $h = h_j = \lambda_j^{-1}$ so that they are rescaled to have length 1 in the interior, and therefore length $\leq 1$ restricted to the boundary.

The difference can be explained because the 'boundary value' of a Dirichlet eigenfunction is the normal derivative, and the semiclassical normal derivative $ihd_n$ has symbol equal to $(1 - |\eta|^2)^{1/2}$ on the characteristic variety, since

$$h^2\Delta - 1 = -h^2 d_n^2 + h^2 \Delta_{\partial\Omega} - 1 + \text{ l.o.t.s, at } \partial\Omega. \tag{9}$$

Since the boundary values appear quadratically in the expectation value, it is not surprising that the ratio between the Dirichlet and Neumann distributions is $1 - |\eta|^2$.

**Moral:** semiclassically, the 'Neumann' analogue of $u$

$$\text{at the boundary is not } d_n u\text{, but } (1 - h^2\Delta_{\partial\Omega})_+^{-1/2} d_n u, \tag{10}$$

where $\Delta_{\partial\Omega}$ is the Laplacian on the boundary.

To see what is wrong with using the naive measure $t_{\mathrm{ld}}$ of the 'boundary condition error', follow the same reasoning as the Dirichlet case to show that

$$(\min t_{\mathrm{ld}}[u])^{-2} = \Big\| \sum_j \frac{w_j \langle w_j, \cdot \rangle}{(\mu^2 - \mu_j^2)^2} \Big\|, \quad E = \mu^2,$$

where $w_j$ is the restriction of the $j$th Neumann eigenfunction $v_j$ to the boundary and $\mu_j^2$ is the eigenvalue. The problem is that the $w_j$ do not behave as uniformly as the $\psi_j$ (normal derivatives of Dirichlet eigenfunctions); we have a lower bound

$$\|w_j\|_{L^2(\partial\Omega)} \geq c, \tag{11}$$

but the sharp upper bound is (Tataru)

$$\|w_j\|_{L^2(\partial\Omega)} \leq C\mu_j^{1/3}. \tag{12}$$

The reason why, in Theorem 2, we were able to get upper and lower bounds on $d(E, \mathrm{spec}_D)$ of the same order in $E$ was that the *lower* bound on the operator norm of a *single* term $\psi_j \langle \psi_j, \cdot \rangle$ was of the same order as the *upper* bound on the sum $\sum_j \psi_j \langle \psi_j, \cdot \rangle$ *over a whole spectral cluster* $|\lambda - \lambda_j| \leq 1$. In the Neumann case, using $t_{\mathrm{ld}}$ will lead to a gap of at least $\mu^{1/3} = E^{1/6}$ between the upper and lower bounds on $d(E, \mathrm{spec}_N)$.

- If we take our **Moral**, (10), seriously, then we could expect to find good upper and lower bounds on the quantity $(1 - h_j^2 \Delta_{\partial\Omega})_+^{1/2} w_j$ instead. Indeed, this is the case:

## Theorem

*Let $\Omega \subset \mathbb{R}^n$ be a smooth bounded domain, and let $w_j$ be the restriction to $\partial\Omega$ of the $j$th $L^2$-normalized Neumann eigenfunction $v_j$. Then there are constants $c, C$ such that*

*(i)* $\| (1 - h_j^2 \Delta_{\partial\Omega})_+^{1/2} w_j \|_{L^2(\partial\Omega)} \geq c, \ \ h_j = \mu_j^{-1};$

*(ii) the operator norm of*

$$\sum_{\mu_j \in [\mu, \mu+1]} (1 - h^2 \Delta_{\partial\Omega})_+^{1/2} w_j \, \langle (1 - h^2 \Delta_{\partial\Omega})_+^{1/2} w_j, \cdot \rangle, \quad h = \mu^{-1},$$

*is bounded by $C$.*

Example: for the unit disc, eigenfunctions have the form

$$v(r,\theta) = ce^{in\theta} J_n(\mu_{n,l} r), \quad J_n'(\mu_{n,l}) = 0,$$

and from (2) we derive

$$2\mu_{n,l}^2 = \int_{\partial\Omega} (\mu_{n,l}^2 - n^2)|v|^2 \implies \|(1 - \Delta_{\partial\Omega}/\mu_j^2)_+^{1/2} w_j\| = \sqrt{2}.$$

Note that when $l = 1$, $\mu_{n,1} \sim n + cn^{1/3}$, and then $\|w_j\| \sim \mu_j^{1/3}$.
These are ‘whispering gallery modes’.

The proof of the upper bound is as follows. We return to (2), and deduce from it that

$$\int_{\partial\Omega} v_j d_n^2 v_j = O(\mu_j^2).$$

It follows, using $(\Delta - \mu_j^2) v_j = 0$ at $\partial\Omega$, and (9), that

$$\int_{\partial\Omega} w_j ((1 - h_j^2 \Delta_{\partial\Omega}) w_j) = O(1).$$

That is,

$$\|(1 - h_j^2 \Delta_{\partial\Omega})_+^{1/2} w_j\|_{L^2(\partial\Omega)}^2 - \|(h_j^2 \Delta_{\partial\Omega} - 1)_+^{1/2} w_j\|_{L^2(\partial\Omega)}^2 = O(1).$$

So it remains to show that the term

$$\|(h_j^2 \Delta_{\partial\Omega} - 1)_+^{1/2} w_j\|_{L^2(\partial\Omega)}^2 \text{ is } O(1) \quad \text{(cf. (8)).}$$

This can be proved by using the characterization $w_j = -2D^t w_j$ where $D$ is the double layer potential at energy $\mu_j^2$, and using the characterization of $D$ from H.-Zelditch that $D$ is an FIO of order zero in the hyperbolic region, namely where $|\eta| \leq 1$, and a pseudodifferential operator of order $-1$ in the elliptic region $\{|\eta| > 1\}$, where $\eta \in T^*(\partial\Omega)$.

- Our argument requires some use of symbol classes which are not coordinate invariant.

Using this theorem as a crucial tool we propose the following MPS for Neumann eigenfunctions: we minimize the quantity

$$t_F[u] = \frac{\|F(\Delta_{\partial\Omega})(d_n u)\|_{L^2(\partial\Omega)}}{\|u\|_{L^2(\Omega)}}, \tag{13}$$

where (cf. **Moral**) (10); also cf. (12)

$$F(\Delta_{\partial\Omega}) = \begin{cases} \left(1 - \frac{\Delta_{\partial\Omega}}{\mu^2}\right)^{-1/2}, & \Delta_{\partial\Omega} \le \mu^2 - \mu^{4/3} \\ \mu^{1/3}, & \Delta_{\partial\Omega} \ge \mu^2 - \mu^{4/3}. \end{cases}$$

This leads to the identity

$$(\min t_F[u])^{-2} = \Big\| \sum_j \frac{F(\Delta_{\partial\Omega})^{-1} w_j \langle F(\Delta_{\partial\Omega})^{-1} w_j, \cdot \rangle}{(\mu^2 - \mu_j^2)^2} \Big\|, \qquad (14)$$

and since $F(\Delta_{\partial\Omega})^{-1}$ is essentially $(1 - h^2 \Delta_{\partial\Omega})_+^{1/2}$, we can use Theorem 3 (together with (12)) to prove the following:

**Theorem**

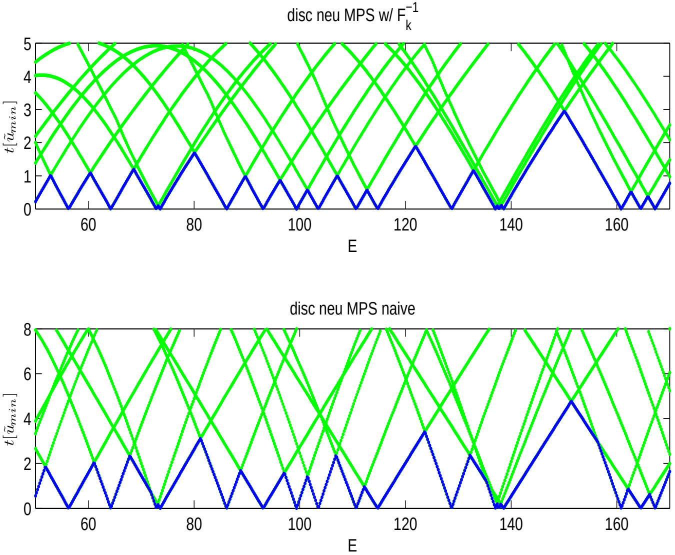
*There exist constants $c, C$ depending only on $\Omega$ such that the following holds. Let $u$ be a nonzero solution of $(\Delta - \mu^2)u = 0$ in $C^\infty(\Omega)$. Let $t_F[u]$ be as in* (13), *and let $u_{\min}$ be the Helmholtz solution minimizing $t_F[u]$. Then*

$$c t_F[u_{\min}] \le d(\mu^2, \mathrm{spec}) \le C t_F[u].$$

A few words about why (14) holds. As before, $(\min t_F[u])^{-1}$ is the operator norm of the composite function $g \mapsto f \mapsto u$, where $f = F(\Delta_{\partial\Omega})^{-1} g$ and $u$ is the Helmholtz solution with $d_n u = f$. We have

$$u = \frac{\sum_j \langle f, w_j \rangle v_j}{\mu^2 - \mu_j^2} = \frac{\sum_j \langle F(\Delta_{\partial\Omega})^{-1} g, w_j \rangle v_j}{\mu^2 - \mu_j^2}$$
$$= \frac{\sum_j \langle g, F(\Delta_{\partial\Omega})^{-1} w_j \rangle v_j}{\mu^2 - \mu_j^2}.$$

Then a $T^*T$ argument gives (14).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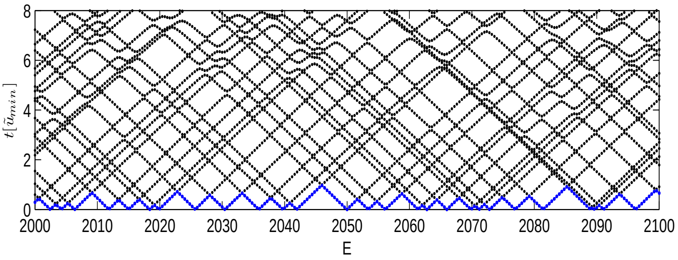
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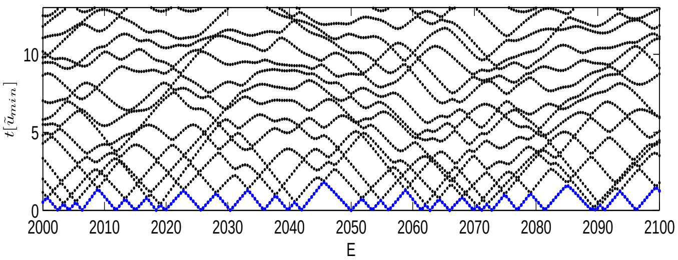
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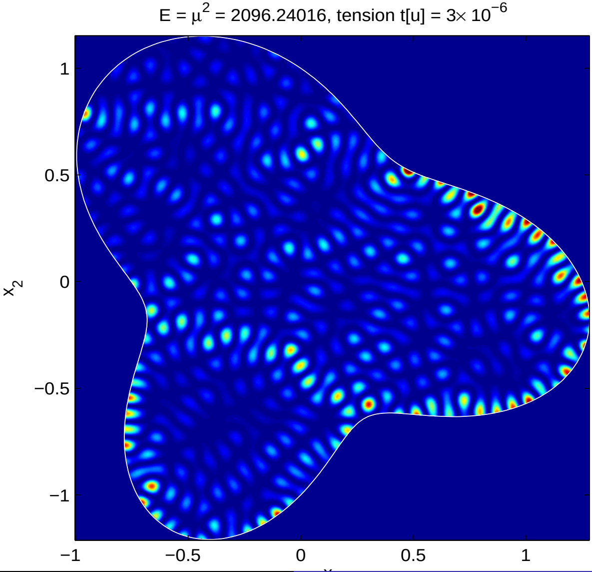
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