Two-parameter localization for eigenfunctions of a Schrödinger operator in balls/spherical shells

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Brief Review of Laplacian eigenvalue problem

Consider the following Laplacian eigenvalue problem with the Dirichlet boundary condition:

$$\begin{cases} -\triangle u = \lambda u \quad \text{in } \Omega, \\ u = 0 \quad \text{on } \partial\Omega, \end{cases}$$

where Ω is a bounded domain in $\mathbb{R}^d$ with a smooth boundary.

The localization behavior of Laplacian eigenvectors strongly depends on the geometry of the domain Ω:

- Ω is a rectangle
- Ω is a ball/spherical shell
- Ω is a sector/annulus sector
- Ω is an ellipse/elliptical sector

Grebenkov, D. S. & Nguyen, B.-T. Geometrical structure of Laplacian eigenfunctions. SIAM Review 55, 601-667 (2013).

Laplacian eigenfunctions in balls

Consider the case where the domain is the unit ball centered at the origin:

$$\Omega_{\mathrm{ball}} = \{x \in \mathbb{R}^d : |x| < 1\}.$$

In spherical coordinates, all basis eigenfunctions of the Laplacian can be represented as

$$u_{klm}(r, \xi) = r^{1-\frac{d}{2}} J_{\nu_l}(j_{\nu_l,k} r) Y_{lm}(\xi),$$

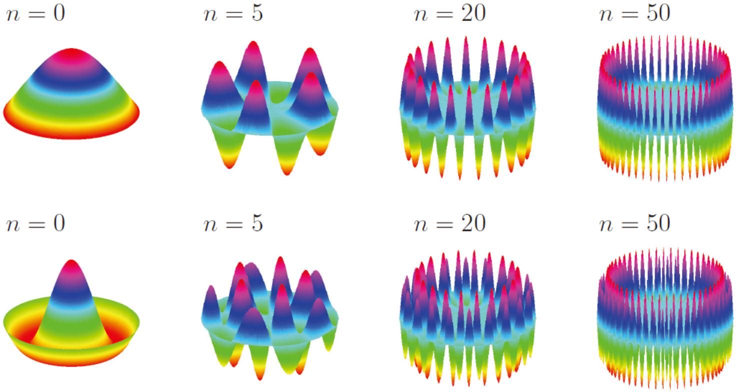
where

- r is the radial coordinate
- ξ is the angular coordinate
- k is the principal quantum number
- l is the azimuthal quantum number
- m is the magnetic quantum number

Nguyen, B.-T. & Grebenkov, D. S. Localization of Laplacian eigenfunctions in circular, spherical, and elliptical domains. SIAM J. Appl. Math. 73, 780-803 (2013).

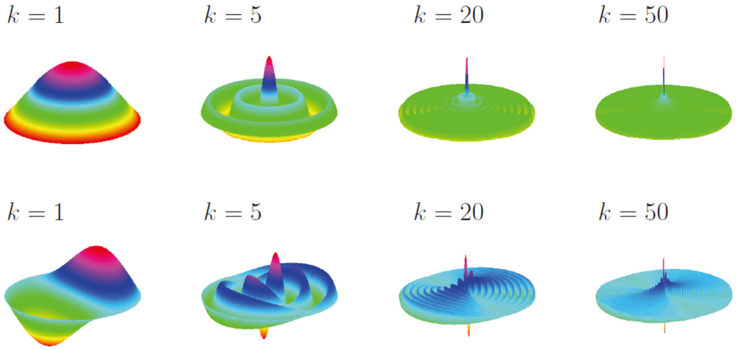
Whispering gallery modes for Laplacian eigenfunctions

The eigenfunctions are localized around the boundary of the ball as the azimuthal quantum number (n) $l \to \infty$ and the principal quantum number k is fixed.



Focusing modes for Laplacian eigenfunctions

The eigenfunctions are localized around the center of the ball as the principal quantum number $k \to \infty$ and the azimuthal quantum number l is fixed.



Questions

Three important questions:

- generalization to other elliptic operators
- generalization to other domains
- phase transition from the whispering gallery modes to focusing modes

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Schrödinger operator with an inverse square potential

Consider the eigenfunctions of the Schrödinger operator

$$Lu = -\triangle u + \frac{c^2}{|x|^2} u$$

with a singular inverse square potential, where $c \geq 0$ is the strength of the potential. Here we focus on the case of $d \geq 2$.

Consider the following eigenvalue problem with the Dirichlet boundary condition:

$$\begin{cases} Lu = \lambda u & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

where Ω is a bounded region in $\mathbb{R}^d$ with a smooth boundary.

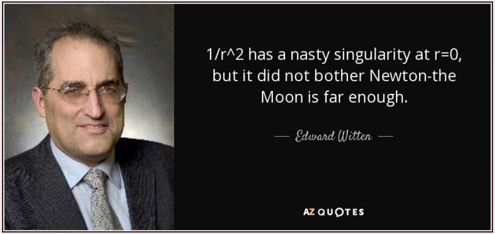
Why do we study the inverse square potential?

Physically, the inverse square potential serves as an intermediate threshold between regular potentials and singular potentials in nonrelativistic quantum mechanics.

Case, K. Singular potentials. Phys. Rev. 80, 797 (1950).

It also arises in many other scientific fields such as nuclear physics, molecular physics, and quantum cosmology.

Frank, W. M., Land, D. J. & Spector, R. M. Singular potentials. Rev. Mod. Phys. 43, 36 (1971).



Define the Sobolev spaces

$$W^1(\Omega) = H^1(\Omega) \cap L^2_{r^{-2}}(\Omega), \quad W^1_0(\Omega) = H^1_0(\Omega) \cap L^2_{r^{-2}}(\Omega)$$

equipped with the norm $\|u\|_{W^1(\Omega)} = (\|\nabla u\|^2 + \|u\|^2_{r^{-2}})^{1/2}$.

Then the variational form of the eigenvalue problem is to find a real number $\lambda \in \mathbb{R}$ and a nonzero function $u \in W^1_0(\Omega) \setminus \{0\}$ such that

$$(\nabla u, \nabla v)_\Omega + c^2 (u, v)_{r^{-2},\Omega} = \lambda (u, v)_\Omega, \quad v \in W^1_0(\Omega).$$

By the Sturm-Liouville theory, all eigenvalues can be listed as

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

Moreover, it is known that that $\lambda_n = O(n^{2/d})$ for any fixed $c \geq 0$.

H. Weyl, Ueber die asymptotische verteilung der eigenwerte, Nachr. Ges. Wiss. Göttingen Math. Phys. Kl., 1911 (1911), pp. 110-117.

Schrödinger eigenvalue problem in balls

Consider the case where the domain is the unit ball centered at the origin:

$$\Omega_{\mathrm{ball}} = \{x \in \mathbb{R}^d : |x| < 1\}.$$

In spherical coordinates, the Laplacian can be written as

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{d-1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Delta_0$$

where $r = |x|$ is the radial coordinate and Δ_0 is the Laplace-Beltrami operator on the sphere S^{d-1}.

The eigenfunctions of the spherical Laplacian Δ_0 are spherical harmonics of degree $l = 0, 1, 2, \cdots$. For each $l \geq 0$, we have

$$\Delta_0 f = -l(l+d-2)f, \quad f \in H_l,$$

where H_l is the vector space of spherical harmonics of degree l.

Spherical coordinates

In spherical coordinates, the eigenvalue problem can be rewritten as

$$\frac{\partial^2 u}{\partial r^2} + \frac{d-1}{r}\frac{\partial u}{\partial r} + \left(\lambda + \frac{\Delta_0 - c^2}{r^2}\right) u = 0.$$

We now represent the eigenfunction u in variable separation form as

$$u(x) = v(r) Y_{lm}(\xi)$$

where r is the radial coordinate, $\xi = (\xi_1, \cdots, \xi_{d-1})$ are angular coordinates, and Y_{lm} are spherical harmonics.

It is easy to check that the radial part $v(r)$ satisfies the second-order ordinary differential equation

$$\frac{\partial^2 v}{\partial r^2} + \frac{d-1}{r}\frac{\partial v}{\partial r} + \left(\lambda - \frac{l(l+d-2) + c^2}{r^2}\right) v = 0.$$

Radial part in balls

We then define a new variable $t = \sqrt{\lambda} r$ and set $\hat{v}(t) = r^{\frac{d}{2}-1} v(r)$. Then the new function $\hat{v}$ turns out to be the solution of the Bessel equation

$$t^2 \frac{\partial^2 \hat{v}}{\partial t^2} + t \frac{\partial \hat{v}}{\partial t} + (t^2 - \nu_l^2)\hat{v} = 0,$$

where

$$\nu_l = \sqrt{\left(l + \frac{d}{2} - 1\right)^2 + c^2}.$$

The radial part

$$v(r) = r^{1-\frac{d}{2}} J_{\nu_l}(\sqrt{\lambda} r),$$

is an ultraspherical Bessel function, where J_{ν_l} is the Bessel function of the first kind of order ν_l.

With this expression, the Dirichlet boundary condition is converted into

$$J_{\nu_l}(\sqrt{\lambda}) = 0.$$

For each $l \geq 0$, the eigenvalue problem has infinitely many positive eigenvalues

$$\lambda_{lk} = j_{\nu_l,k}^2, \quad k = 1, 2, \cdots,$$

where $j_{\nu_l,k}$ is the kth zero of the Bessel function J_{ν_l}.

Finally, all basis eigenfunctions of the eigenvalue problem can be represented as

$$u_{klm}(r,\xi) = r^{1-\frac{d}{2}} J_{\nu_l}(j_{\nu_l,k} r) Y_{lm}(\xi),$$

where

- k is the principal quantum number
- l is the azimuthal quantum number
- m is the magnetic quantum number

Two-parameter asymptotic behavior for the zeros

Previous studies:

One-parameter high-frequency localization for Laplacian eigenfunctions as $l \to \infty$ and k is fixed or as $k \to \infty$ and l is fixed.

Our work:

Two-parameter high-frequency localization for Schrödinger eigenfunctions as $l, k \to \infty$ simultaneously while keeping $l/k \to w$.

Lemma

As $l, k \to \infty$ while keeping $l/k \to w > 0$, we have

$$\frac{j_{\nu_l,k}}{\nu_l} \to h(w),$$

where $h(w) > 1$ is the unique solution of the algebraic equation

$$\sqrt{h(w)^2 - 1} - \operatorname{arcsec}(h(w)) = \frac{\pi}{w}.$$

Two-parameter L^∞- and L^p-localization

Two-parameter L^∞-localization for eigenfunctions in balls:

Theorem

For any $r > 0$ and $\epsilon > 0$, let $D(r,\epsilon) = \{x \in \mathbb{R}^d : ||x| - r| \geq \epsilon\}$. Then for any $\epsilon > 0$, as $l, k \to \infty$ while keeping $l/k \to w > 0$, we have

$$\frac{\|u_{klm}\|_{L^\infty(D(1/h(w),\epsilon))}}{\|u_{klm}\|_{L^\infty(\Omega_{ball})}} \to 0.$$

Two-parameter L^p-localization for eigenfunctions in balls:

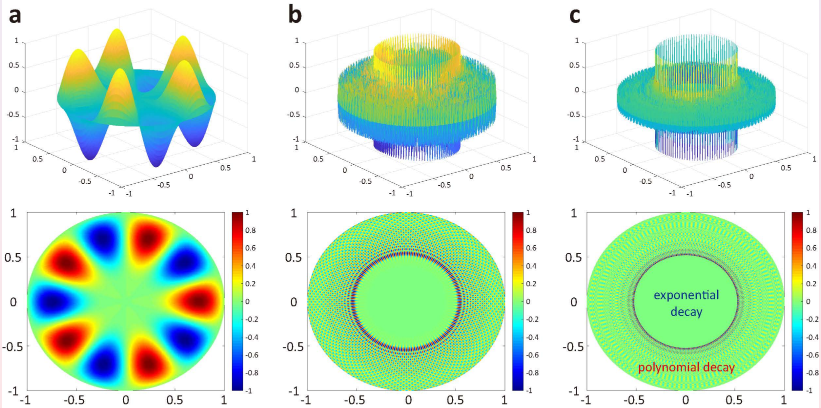
Theorem

The notation is the same as in the above theorem. Then for any $\epsilon > 0$ and $p > 4$, as $l, k \to \infty$ while keeping $l/k \to w > 0$, we have

$$\frac{\|u_{klm}\|_{L^p(D(1/h(w),\epsilon))}}{\|u_{klm}\|_{L^p(\Omega_{ball})}} \to 0.$$

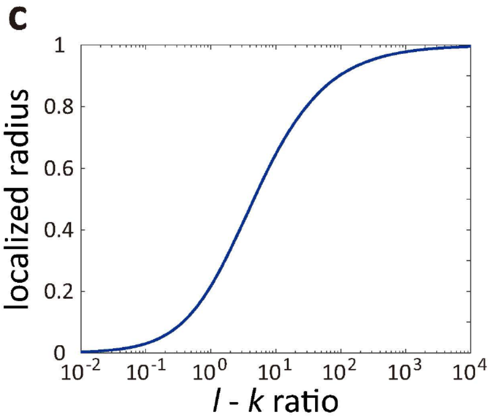
Novel localization behavior

As $l, k \to \infty$ while keeping $l/k \to w > 0$, the eigenfunctions are localized around an intermediate sphere with radius $1/h(w) \in (0, 1)$.



Localized radius

With the increase of the *l*-*k* ratio w, the localized radius $1/h(w)$ also increases.



Decaying speed

Exponential decay inside the localized radius:

$$\frac{\|u_{klm}\|_{L^\infty(D_1(1/h(w),\epsilon))}}{\|u_{klm}\|_{L^\infty(\Omega_{\mathrm{ball}})}} \lesssim q^{\nu_l+1-d/2} \to 0.$$

For any $p \geq 1$, we have

$$\frac{\|u_{klm}\|^p_{L^p(D_1(1/h(w),\epsilon))}}{\|u_{klm}\|^p_{L^p(\Omega_{\mathrm{ball}})}} \lesssim \nu_l^{(p+2)/3} J_{\nu_l}(\nu_l)^p q^{p\nu_l+\alpha} \lesssim \nu_l^{2/3} q^{p\nu_l+\alpha} \to 0.$$

Polynomial decay outside the localized radius:

$$\frac{\|u_{klm}\|_{L^\infty(D_2(1/h(w),\epsilon))}}{\|u_{klm}\|_{L^\infty(\Omega_{\mathrm{ball}})}} \lesssim \nu_l^{-1/6} \to 0.$$

For any $p > 4$, we have

$$\frac{\|u_{klm}\|^p_{L^p(D_2(1/h(w),\epsilon))}}{\|u_{klm}\|^p_{L^p(\Omega_{\mathrm{ball}})}} \lesssim \nu_l^{(p+2)/3-p/2} \to 0.$$

Reduction to the whispering gallery mode

As $l \to \infty$ and k is fixed, we have $l/k \to \infty$.

In the limiting case of $w \to \infty$, the localized radius $1/h(w) \to 1$ and thus the eigenfunctions are localized around the boundary of the ball, giving rise to whispering gallery modes.

Corollary

For any $\epsilon > 0$, let $A(\epsilon) = \{x \in \mathbb{R}^d : |x| \leq 1 - \epsilon\}$. Then for any $\epsilon > 0$ and $1 \leq p \leq \infty$, we have

$$\lim_{l \to \infty} \frac{\|u_{klm}\|_{L^p(A(\epsilon))}}{\|u_{klm}\|_{L^p(\Omega_{ball})}} = 0.$$

Reduction to the focusing mode

As $k \to \infty$ and l is fixed, we have $l/k \to 0$.

In the limiting case of $w \to 0$, the localized radius $1/h(w) \to 0$ and thus the eigenfunctions are localized around the center of the ball, giving rise to focusing modes.

Corollary

For any $\epsilon > 0$, let $B(\epsilon) = \{x \in \mathbb{R}^d : \epsilon \leq |x| \leq 1\}$. Then for any $\epsilon > 0$ and

$$\frac{2d}{d-1} < p \leq \infty,$$

we have

$$\lim_{k \to \infty} \frac{\|u_{klm}\|_{L^p(B(\epsilon))}}{\|u_{klm}\|_{L^p(\Omega_{ball})}} = 0.$$

Quantum mechanistic picture

As the azimuthal quantum number l increases, the angular momentum of the particle also increases, which throws the particle outwards and thus induces localization around the boundary.

Since the inverse square potential $V(x) = c^2/|x|^2$ corresponds to an expulsive force, the energy of the particle is high when it is close to the origin and is low when it is far away from the origin. As the principal quantum number k increases, the energy of the particle also increases, which pulls the particle towards the origin and thus induces localization around the center.

Schrödinger eigenvalue problem in spherical shells

Consider the case where the domain is a spherical shell:

$$\Omega_{\text{shell}} = \{x \in \mathbb{R}^d : 1 < |x| < R\},$$

We now represent the eigenfunction u in variable separation form as

$$u(x) = v(r) Y_{lm}(\xi)$$

where r is the radial coordinate, $\xi = (\xi_1, \cdots, \xi_{d-1})$ are angular coordinates, and Y_{lm} are spherical harmonics.

It is easy to check that the radial part $v(r)$ satisfies the second-order ordinary differential equation

$$\frac{\partial^2 v}{\partial r^2} + \frac{d-1}{r}\frac{\partial v}{\partial r} + \left(\lambda - \frac{l(l+d-2)+c^2}{r^2}\right) v = 0.$$

Radial part in spherical shells

The radial part

$$v(r) = r^{1-\frac{d}{2}}[\alpha J_{\nu_l}(\sqrt{\lambda}r) + \beta Y_{\nu_l}(\sqrt{\lambda}r)].$$

where J_{ν_l} and Y_{ν_l} are Bessel functions of the first and second kinds of order ν_l, respectively.

With this expression, the Dirichlet boundary condition is converted into the system of linear equations

$$\begin{cases} \alpha J_{\nu_l}(\sqrt{\lambda}) + \beta Y_{\nu_l}(\sqrt{\lambda}) = 0, \\ \alpha J_{\nu_l}(\sqrt{\lambda}R) + \beta Y_{\nu_l}(\sqrt{\lambda}R) = 0. \end{cases}$$

Since α and β are not simultaneously zero, the coefficient matrix of the above system of linear equations is not invertible, that is,

$$J_{\nu_l}(\sqrt{\lambda})Y_{\nu_l}(\sqrt{\lambda}R) - Y_{\nu_l}(\sqrt{\lambda})J_{\nu_l}(\sqrt{\lambda}R) = 0.$$

For each $l \geq 0$, the eigenvalue problem has infinitely many positive eigenvalues

$$\lambda_{lk} = a^2_{\nu_l,k}, \quad k = 1, 2, \cdots ,$$

where $a_{\nu_l,k}$ is the kth zero of the cross product

$$f_{\nu_l,R}(z) = J_{\nu_l}(z) Y_{\nu_l}(Rz) - Y_{\nu_l}(z) J_{\nu_l}(Rz).$$

Finally, all basis eigenfunctions of the eigenvalue problem can be represented as

$$u_{klm}(r, \xi) = r^{1-\frac{d}{2}} F_{\nu_l,k}(a_{\nu_l,k} r) Y_{lm}(\xi),$$

where

$$F_{\nu_l,k}(z) = J_{\nu_l}(a_{\nu_l,k}) Y_{\nu_l}(z) - Y_{\nu_l}(a_{\nu_l,k}) J_{\nu_l}(z)$$

is a cylinder function, which is defined as a linear combination of Bessel functions of the first and second kinds.

Two-parameter asymptotic behavior for the zeros

Lemma

As $l, k \to \infty$ while keeping $l/k \to w > 0$, we have

$$\frac{a_{\nu_l,k}}{\nu_l} \to \frac{g_R(w)}{w},$$

where $g_R(w)$ is the unique solution of the initial value problem

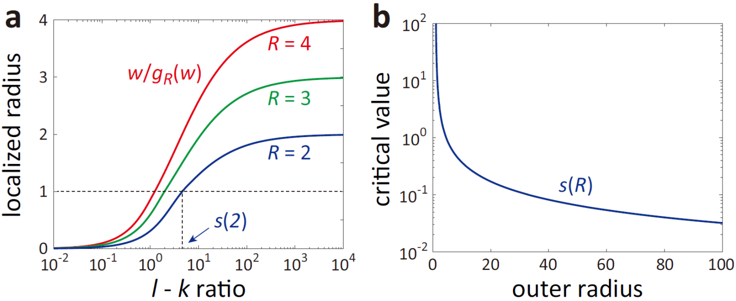
$$\frac{dy}{dw} = \frac{\arccos\left(\frac{w}{Ry}\right) - \arccos\left(\frac{w}{y}\right) I_{\{|w|\le|y|\}}}{R\sqrt{1-\left(\frac{w}{Ry}\right)^2} - \sqrt{1-\left(\frac{w}{y}\right)^2} I_{\{|w|\le|y|\}}}, \quad y(0) = \frac{\pi}{R-1}.$$

Moreover, both $g_R(w)$ and $w/g_R(w)$ are strictly increasing on $(0,\infty)$ with

$$\lim_{w\to 0}\frac{w}{g_R(w)} = 0, \quad \lim_{w\to\infty}\frac{w}{g_R(w)} = R.$$

Existence of the critical value

The function $w/g_R(w)$ versus the outer radius $R > 1$:

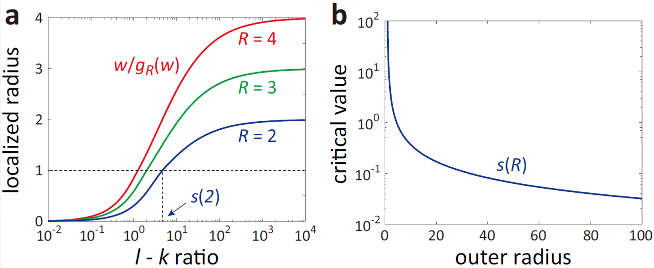


Since it is a strictly increasing function ranging from 0 to R, there must exist a unique critical value $s(R) > 0$ such that

$$g_R(s(R)) = s(R).$$

Properties of the critical value

The function $s(R)$ versus the outer radius $R > 1$:



Lemma

$s(R)$ is a strictly decreasing function of R. Moreover, $s(R)$ has the following limit behavior:

$$\lim_{R\to 1+} s(R) = \infty, \quad \lim_{R\to\infty} s(R) = 0.$$

Paris-type inequality for cylinder functions

Lower bound of the Paris-type inequality for cylinder functions:

Laforgia, A. Inequalities for Bessel functions. J. Comput. Appl. Math. 15, 75-81 (1986).

Upper bound of the Paris-type inequality for cylinder functions:

Lemma

Suppose that $l/k \to w > s(R)$ as $l, k \to \infty$. When l is sufficiently large, we have

$$0 \leq \frac{F_{\nu_l,k}(\nu_l z)}{z^{\nu_l} F_{\nu_l,k}(\nu_l)} \leq e^{\frac{\nu_l^2(1-z^2)}{2(\nu_l+1)}} \leq e^{\nu_l(1-z)}, \quad \frac{a_{\nu_l,k}}{\nu_l} \leq z \leq 1.$$

Two-parameter L^p-localization

Two-parameter L^∞-localization for eigenfunctions in spherical shells:

Theorem

For any $r > 0$ and $\epsilon > 0$, let $D(r, \epsilon) = \{x \in \mathbb{R}^d : ||x| - r| \geq \epsilon\}$. Then for any $\epsilon > 0$, as $l, k \to \infty$ while keeping $l/k \to w > s(R)$, we have

$$\frac{\|u_{klm}\|_{L^\infty(D(w/g_R(w),\epsilon))}}{\|u_{klm}\|_{L^\infty(\Omega_{shell})}} \to 0.$$

Two-parameter L^p-localization for eigenfunctions in spherical shells:

Theorem

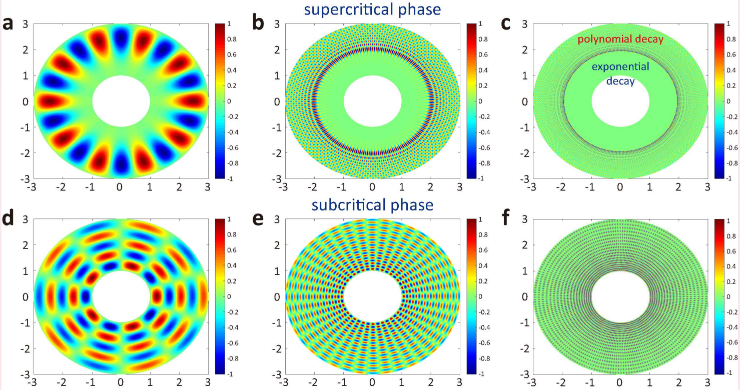
The notation is the same as in the above theorem. Then for any $\epsilon > 0$ and $p > 4$, as $l, k \to \infty$ while keeping $l/k \to w > s(R)$, we have

$$\frac{\|u_{klm}\|_{L^p(D(w/g_R(w),\epsilon))}}{\|u_{klm}\|_{L^p(\Omega_{shell})}} \to 0.$$

Phase transition

Phase transition when the l-k ratio w crosses its critical value $s(R)$:

- Supercritical case of $w > s(R)$: localized around an intermediate sphere with radius $w/g_R(w) \in (1, R)$
- Subcritical case of $w < s(R)$: localization fails to be observed



Localization index

To further understand the phase transition, we introduce a quantity called the localization index, which is defined as

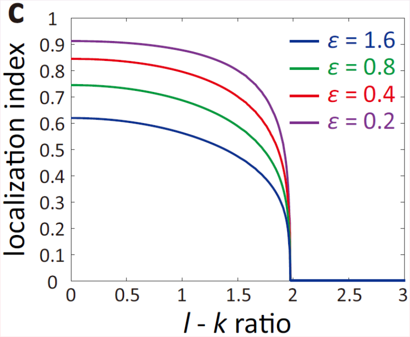
$$\gamma_{R,\epsilon}(w) = \begin{cases} \lim\limits_{l,k\to\infty} \dfrac{\|u_{klm}\|_{L^\infty(D(w/g_R(w),\epsilon))}}{\|u_{klm}\|_{L^\infty(\Omega_{\mathrm{shell}})}}, & w > s(R), \\ \lim\limits_{l,k\to\infty} \dfrac{\|u_{klm}\|_{L^\infty(D(1,\epsilon))}}{\|u_{klm}\|_{L^\infty(\Omega_{\mathrm{shell}})}}. & w \le s(R). \end{cases}$$

Clearly, this is a number between 0 and 1 and is equal to 0 in the supercritical case of $w > s(R)$.

Second-order phase transition

Second-order phase transition as w crosses its critical value $s(R)$:

- w serves as the tuning parameter
- $\gamma_{R,\epsilon}(w)$ serves as the order parameter
- l or k serves as the system size



Whispering gallery modes and the breaking of focusing modes

The eigenfunctions are localized around the outer boundary of the spherical shell as $l \to \infty$ and k is fixed $(w = \infty)$, giving rise to whispering gallery modes.

Corollary

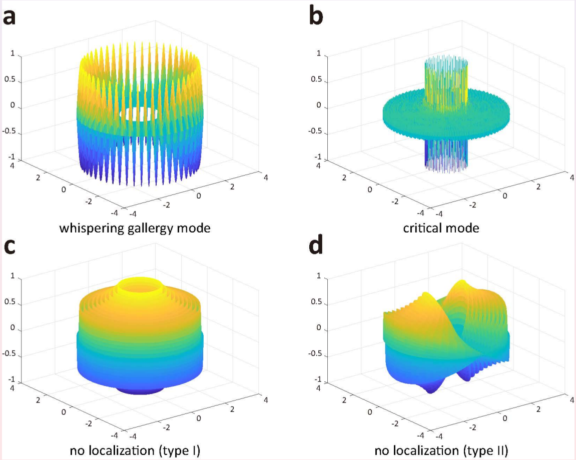
For each $\epsilon > 0$, let $A_R(\epsilon) = \{x \in \mathbb{R}^d : 1 \le |x| \le R - \epsilon\}$. Then for any $\epsilon > 0$ and $1 \le p \le \infty$, we have

$$\lim_{l \to \infty} \frac{\|u_{klm}\|_{L^p(A_R(\epsilon))}}{\|u_{klm}\|_{L^p(\Omega_{shell})}} = 0.$$

The eigenfunctions fail to localize as $k \to \infty$ and l is fixed $(w = 0)$, giving rise to localization breaking.

Critical modes

The eigenfunctions are localized around the outer boundary of the spherical shell in the critical case of $w = s(R)$, leading to critical modes.



Two-parameter localization in sectors

Consider the case where the domain Ω is a sector with polar coordinate representation:

$$\Omega = \{(r, \theta) : r < 1,\ 0 < \theta < \beta\pi\},$$

where $0 < \beta < 2$.

Similarly, all basis eigenfunctions of the eigenvalue problem are given by

$$u_{kl}(r, \xi) = J_{\nu_l}(j_{\nu_l,k} r) \sin\left(\frac{l\theta}{\beta}\right),$$

where $\nu_l = \sqrt{l^2 + c^2}$ and $j_{\nu_l,k}$ is the kth zero of the Bessel function J_{ν_l}.

As $k, l \to \infty$ while keeping $l/k \to w > 0$, the eigenfunctions are localized around the circular arc with polar coordinate representation

$$\{(r, \theta) : r = 1/h(w),\ 0 < \theta < \beta\pi\}.$$

Moreover, whispering gallery modes appear as $l \to \infty$ and k is fixed and focusing modes appear as $k \to \infty$ and l is fixed.

Two-parameter localization in annulus sectors

Consider the case where the domain Ω is an annulus sector with polar coordinate representation

$$\Omega = \{(r,\theta) : 1 < r < R,\ 0 < \theta < \beta\pi\},$$

where $R > 1$ and $0 < \beta < 2$.

Similarly, all basis eigenfunctions of the eigenvalue problem are given by

$$u_{kl}(r,\xi) = [J_{\nu_l}(a_{\nu_l,k})Y_{\nu_l}(a_{\nu_l,k}r) - Y_{\nu_l}(a_{\nu_l,k})J_{\nu_l}(a_{\nu_l,k}r)]\sin\left(\frac{l\theta}{\beta}\right).$$

where $a_{\nu_l,k}$ is the kth zero of the cross product $f_{\mu_l,R}$.

As $k, l \to \infty$ while keeping $l/k \to w > 0$, the eigenfunctions undergo a phase transition as the l-k ratio w crosses the critical value $s(R)$.

The whispering gallery modes appear as $l \to \infty$ and k is fixed, while the focusing modes will not appear as $k \to \infty$ and l is fixed.

Thanks for your attention!