An Explicit Formula of the Dirichlet-to-Neumann Map for a Radial Potential in Dimension 3

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Outline

Introduction

- Let us consider a bounded domain $\Omega \subset \mathbb{R}^3$ with smooth boundary, the boundary value problem for the Schrödinger equation in Ω is given as follows

$$\begin{cases} (-\Delta + q)u &= 0 & \text{in } \Omega, \\ u &= f & \text{on } \partial\Omega. \end{cases} \qquad (1)$$

- The boundary value is assumed to be in $H^{1/2}(\partial\Omega)$, and the potential q is real-valued function satisfying $q \in \mathrm{L}^\infty(\Omega)$.

Motivation

Inverse problem for the Schrödinger equation is related to the Calderón's problem see [1, 2].

$$\begin{cases} \nabla.(\gamma\nabla u) = 0, & \text{in } \Omega, \\ u = f & \text{on } \partial\Omega. \end{cases} \tag{2}$$

- Calderón's was motived by oil prospection. It is applied in location of oil and mineral deposits in the Earth's interior.
- Diagnosis of breast cancer.
- Monitoring pulmonary functions.
- Detection leaks in buried pipes, among others.

The study of the problem (2), for $n \geq 3$ and regular γ, is reduced to problem 1 with $q(x) = \dfrac{\Delta \gamma^{1/2}}{\gamma^{1/2}}$, see [3].
That is why we are motivated to study the problem 1.

The inverse problem for the Schrödinger equation is to determine the potential function q from the measurements of $\frac{\partial u}{\partial \nu}$ for all possible functions f on the boundary of Ω. That is the knowledge of the map, called also Dirichlet-to-Neumann map for the Schrödinger equation, that associates to any $f \in H^{1/2}(\partial\Omega)$ the normal derivative, $\frac{\partial u}{\partial \nu} \in H^{-1/2}(\partial\Omega)$, of the unique solution of 1.

In the literature, the spectral geometry of the Dirichlet-to-Neumann map is a new and rapidly developing branch of spectral theory.
The eigenvalue problem for the Dirichlet-to-Neumann map, called the Steklov problems, was first introduced by V. A. Steklov more than a century ago. The geometric properties of Steklov eigenvalues and eigenfunctions have only recently begum to be explored.
Many studies to determine a map related to the Schrödinger operator in quantum mechanics, and to estimate the entropy numbers of the function space have also developed, see [3] and references therein.

Outline

Definition of the Dirichlet-to-Neumann map for the Schrödinger equation

- In this section we define the Dirichlet-to-Neumann map Λ_q for the Schrödinger equation formally as

$$\begin{array}{rccc} \Lambda_q : H^{1/2}(\partial\Omega) & \longrightarrow & H^{-1/2}(\partial\Omega) & \\ f & \longmapsto & \Lambda_q(f) = \frac{\partial u}{\partial \nu}\Big|_{\partial\Omega}, & \end{array} \quad (3)$$

where ν is the outer unit normal vector to $\partial\Omega$.
- The map $f \longmapsto \Lambda_q(f)$ depends linearly on f.
- Λ_q encodes the measurements of $\frac{\partial u}{\partial \nu}$ for all possible functions f on the boundary of Ω.

- We need to assume that 0 is not a Dirichlet eigenvalue of $(-\Delta + q)$ in Ω.
- Now, we look more closely at the direct problem with the potential. Let the unit ball B in $\mathbb{R}^3$ be defined by $B = \left\{x \in \mathbb{R}^3 : |x| \leq 1\right\}$.
- We focus on $q \in \mathrm{L}^{\infty}(B)$ with $q(x) = q(|x|)$ is radial, $f \in H^{\frac{1}{2}}(\partial B)$ given and assuming that 0 is not an eigenvalue of

$$\begin{cases} (-\Delta + q)u = 0 & \text{in } |x| < 1, \\ u = f & \text{on } |x| = 1. \end{cases} \tag{4}$$

- These choices guarantee the existence of a solution of (4) by the Fourier method and 0 is not an eigenvalue ensuring the uniqueness of the solution.
- Then the map $f \longmapsto \Lambda_q(f)$ is well defined.

To obtain an explicit formula for the Dirichlet-to-Neuman map Λ_q defined in (3), we will consider the following results, see (Mueller, Siltanen) :

1. If $q(x) \neq 0$ then Λ_q is diagonalisable in the sense that the spectrum is discrete, $\left\{\lambda_k\left[q\right], k \in \mathbb{N}_0\right\}$.
   In this case, if $\mathcal{N}_k$ is the subspace of spherical harmonics of degree k, then

$$\Lambda_q\big|_{\mathcal{N}_k} = \lambda_k\left[q\right] I_{\mathcal{N}_k}.$$

2. If $q(x) = 0$ and $\phi_k \in \mathcal{N}_k$ then
   $\Lambda_0(\phi_k) = k\phi_k, \quad k = 0, 1, 2, ...$
3. $\lambda_k\left[q\right] - k \longrightarrow 0$ if $k \longrightarrow \infty$.

Then in the following, we give a recurrence relation for the explicit calculation of the spectrum in the case where $q(x)$ is a step potential, to give an approximation of the spectrum of a general potential. For this, we need to introduce some properties that will be useful.

Outline

Radial Solutions

Some results obtained from writing the problem (4) in polar coordinates $r > 0,\ \theta \in \mathbb{S}^2$. We want to obtain "complex geometrical optics" solutions or solutions of Faddeev types.

Lemma

If $v(r,\theta) = u(r\theta)$ then, the function v satisfies :

$$\begin{cases} r^2 v'' + 2rv' + \Delta_S v - q(r) r^2 v = 0, \\ \lim\limits_{r>0,\ r\to 0} v(r,\theta) < \infty, \quad v(1,\theta) = f(\theta). \end{cases} \tag{5}$$

where $-\Delta_S Y_\ell^k = \ell(\ell+1) Y_\ell^k, \qquad Y_\ell^k \in \mathcal{N}_\ell.$

Lemma

If $f(\theta) = \sum_{\ell=0}^{\infty} \sum_{k=-\ell}^{\ell} f_{\ell k} Y_\ell^k(\theta)$ *in* $H^{1/2}(\mathbb{S}^2)$, *then the equation (4) admits a unique solution of the form*

$$v(r,\theta) = \sum_{\ell=0}^{\infty} \sum_{k=-\ell}^{\ell} v_{\ell k}(r) Y_\ell^k(\theta), \tag{6}$$

where $v_{\ell k}$ *satisfies the problem*

$$\begin{cases} r^2 v_{\ell k}'' + 2r v_{\ell k}' - \ell(\ell+1) v_{\ell k} - q(r) r^2 v_{\ell k} = 0, \quad r \in (0,1), \\ \lim\limits_{r>0,\, r\to 0} v_{\ell k}(r) < \infty, \quad v_{\ell k}(1) = f_{\ell k}. \end{cases} \tag{7}$$

Lemma

If $v_{\ell k}$ is the solution of (7), then we have

$$\Lambda_q(f) = \sum_{\ell=0}^{\infty} \sum_{k=-\ell}^{\ell} v'_{\ell k}(1) Y_\ell^k(\theta). \tag{8}$$

Lemma

In (7), if we take $f = Y_\ell$, that is, the spherical harmonic of degree ℓ, it follows that

$$\Lambda_q(Y_\ell)(\theta) = v_\ell'(1)Y_\ell(\theta). \tag{9}$$

Then $v_l'(1)$ is an eigenvalue of Λ_q with multiplicity $2\ell + 1$ and its eigenfunctions are $\{Y_\ell^k\}_{k=-\ell,\, -\ell+1,\cdots,\, \ell-1,\, \ell}$.

Outline

Explicit formula for the Dirichlet-to-Neumann map
The case where q is a piecewise constant radial potential

For all $\ell \in \mathbb{N}$, $p_\ell^m(r)$ denotes the Bessel function of the first type $j_\ell(\sqrt{|\gamma_m|}r)$ or the Bessel function of the second type $i_\ell(\sqrt{|\gamma_m|}r)$, and $q_\ell^m(r)$ denotes the modified Bessel function of the first type $y_\ell(\sqrt{|\gamma_m|}r)$ or the modified Bessel function of the second type $(-1)^{\ell+1}k_\ell(\sqrt{|\gamma_m|}r)$. Let us introduce the theorem where the expression of the Dirichlet-to-Neuman map is presented when q is a piecewise constant radial potential, based on the results of the previous section.

Theorem

Let the unit ball B in $\mathbb{R}^3$ and the scaled potential $q \in \mathrm{L}^\infty(B)$ with

$$q(r) = \sum_{m=1}^{n} \gamma_m \chi_{(r_{m-1},\, r_m)}, \qquad r = |x|, \tag{10}$$

such that the Dirichlet problem for $-\Delta + q$ is well-posed. Then there is an explicit formula for the Dirichlet-to-Neumann map defined as follows :

$$\Lambda_q\left[Y_\ell^k(\theta)\right]=\left[C\left(k_n p_{\ell-1}^n(1)-\frac{k_n p_\ell^n(1)}{q_\ell^n(1)}q_{\ell-1}^n(1)\right)\right.$$

$$\left.+\frac{k_n q_{\ell-1}^n(1)-\ell q_\ell^n(1)}{q_\ell^n(1)}\right]Y_\ell^k(\theta),\ \ell=1,\ 2,\ldots \qquad (11)$$

with C depending on n and ℓ.

For proof, we assume that $\gamma_m \neq 0$ to simplify the calculations. If we want to consider this case in the simulations, we approximate it by $\gamma = -0.01$.
And we use lemmas introduced.

Explicit formula for the Dirichlet-to-Neumann map

The case where the potential q is a continuous radial function

For all $\ell \in \mathbb{N}$, $p_\ell^m(r)$ denotes the Bessel function of the first type $j_\ell(\sqrt{|\gamma_m|}r)$ or the Bessel function of the second type $i_\ell(\sqrt{|\gamma_m|}r)$, and $q_\ell^m(r)$ denotes the modified Bessel function of the first type $y_\ell(\sqrt{|\gamma_m|}r)$ or the modified Bessel function of the second type $(-1)^{\ell+1}k_\ell(\sqrt{|\gamma_m|}r)$. Let us introduce the theorem where the expression of the Dirichlet-to-Neuman map is presented when the potential q is a continuous function with $q(r) > 0$ or $q(r) < 0$ in the interval $[0,\ 1]$, based on the results of a piecewise constant radial potential.

Theorem

Let the unit ball B in $\mathbb{R}^3$ and a continuous radial potential function $q \in \mathrm{L}^\infty(B)$ with $q(r) = q(|x|)$, where $q(r) > 0$ or $q(r) < 0$, such that the Dirichlet problem for $-\Delta + q$ is well posed.
Let n be a large integer number such that $[0,\ 1] = \bigcup_1^n [r_{m-1},\ r_m]$ with $m = 1, \dots, n$ and where $r_0 = 0,\ r_n = 1$ and $r_m - r_{m-1} = \frac{1}{n}$.
Let a denote $k_m = \sqrt{|q(r_m)|}$.
There is, for n enough large integer numbers and $\ell = 1, 2, \dots,$ an explicit formula for the Dirichlet-to-Neumann map defined as follows :

$$\Lambda_q(Y_\ell^k(\theta)) = \left[\widetilde{C} \left(\sqrt{|q(1)|}\, p_{\ell-1}^*(1) - \frac{\sqrt{|q(1)|}\, p_\ell^*(1)}{q_\ell^*(1)} q_{\ell-1}^*(1) \right) + \frac{\sqrt{|q(1)|}\, q_{\ell-1}^*(1) - \ell q_\ell^*(1)}{q_\ell^*(1)} \right] Y_\ell^k(\theta). \qquad (12)$$

With $\widetilde{C}$ depending ℓ, $p_\ell^*(1) = p_\ell(\sqrt{|q(1)|})$,
$p_{\ell-1}^*(1) = p_{\ell-1}(\sqrt{|q(1)|})$,
$q_\ell^*(1) = q_\ell(\sqrt{|q(1)|})$ and $q_{\ell-1}^*(1) = q_{\ell-1}(\sqrt{|q(1)|})$.

For proof, we introduce $q_i, i = 1, 2$ be piecewise constant radial functions, $q_i(r) = q(|x|)$, defined by

$$\begin{aligned} q_1(r) &= \textstyle\sum_{m=1}^{n} q(r_{m-1})\chi_{(r_{m-1}, r_m)}, \\ q_2(r) &= \textstyle\sum_{m=1}^{n} q(r_m)\chi_{(r_{m-1}, r_m)}, r = |x|. \end{aligned} \tag{13}$$

And we use the theorem 4.1.

Outline

Numerical Simulations

In this section, we denote $k = \ell - 1$, and then $k = 0, 1, 2, ...$ when $\ell = 1, 2, ...$, and then we write λ_k in the simulations. We will numerically compute the potential q, λ_k, $k - \lambda_k$, and $\log(|k - \lambda_k|)$, $k = 0, 1, 2, ...$ We will check numerically if the eigenvalues found in theorems (4.1) and (4.2) verify the properties 1 to 3 introduced in section 2.

We consider the case where the radial potential is defined by a piecewise constant function

$$q(r) = \sum_{m=1}^{n} \gamma_m \chi_{(r_{m-1},\, r_m)}, \qquad r = |x|,$$

where $n \geq 1$, γ_m, $r_m \in \mathbb{R}$ with

At the first, we consider two examples of piecewise constant radial potential functions where the length of interval $[r_{m-1},\ r_m]$ is arbitrary.
We denote **Case** 1 the case where the potential value at each interval is a random value between -2 and 0.
Case 2 where the potential value at each interval is a random value between -2 and 2.
Using the results of the above section for these cases, we obtain the following results.

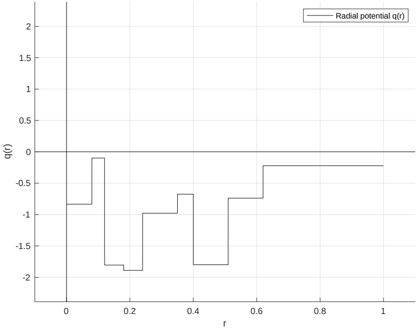

FIGURE – Radial potential in Case 1

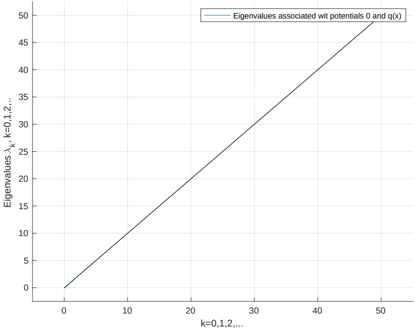

FIGURE – Eigenvalues associated with potential in Case 1

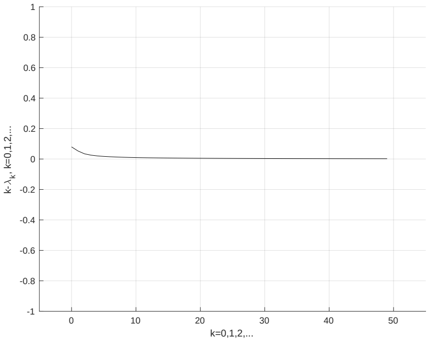

FIGURE – (Eigenvalues-order)-limit in Case 1

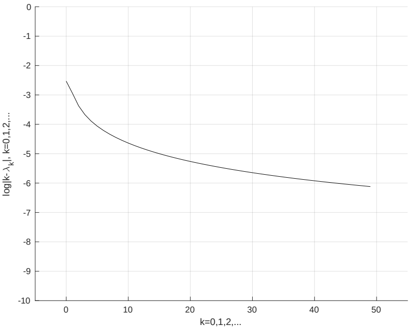

FIGURE – Confirmation eigenvalues limit in Case 1

In Figure 1 there is an example of the potential q and in Figure 2 we see the corresponding eigenvalues. As excepted, we confirm in 3 and 4.
These figures show that the eigenvalues defining the Dirichlet-to-Neuman map in theorem (4.1) verify the 1 to 3 properties considered in **Section 2**.

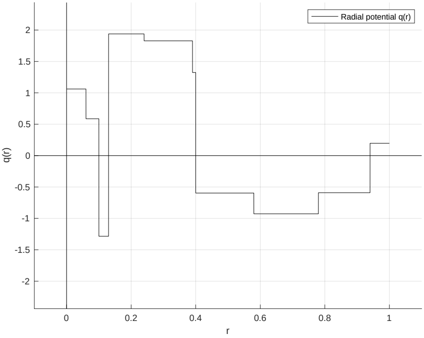

FIGURE – Radial potential in Case 2

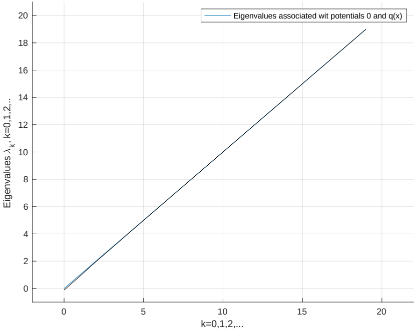

FIGURE – Eigenvalues associated with potentials in Case 2

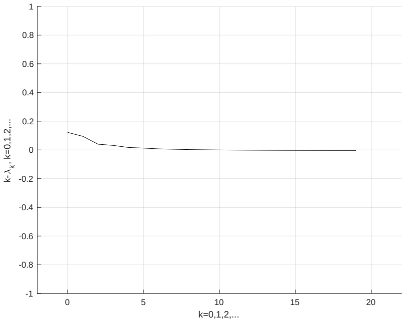

FIGURE – (Eigenvalues-order)-limit in Case 2

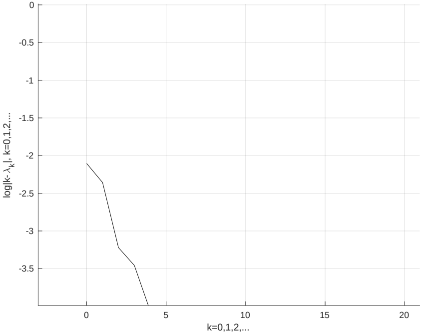

FIGURE – Confirmation eigenvalues limit in Case 2

In Figure 5 there is also an example of the potential q and in Figure 6 we see the corresponding eigenvalues. As excepted, we confirm in 7 and 8.

These figures show that the eigenvalues defining the Dirichlet-to-Neuman map in the theorem (4.1) verify also the 1 to 3 properties considered in **Section 2**.

For potential positives, we only need to take the absolute values of γ_m in Case 2.

Secondly, we consider an example of radial continuous potential function in $[0,\ 1] = \bigcup_1^n [r_{m-1},\ r_m]\,,\ m = 1, ..., n$ where the length of intervals $[r_{m-1},\ r_m]$ is constant and equal to $\frac{1}{n}$.
We denote this example **Case** 3 taking $q(r) = 0.05 + r^2$.
We approximate it by two piecewise constant radial potential functions $q_1(r)$ and $q_2(r)$ such that $q_1(r) \leq q(r) \leq q_2(r)$.
Using the results of the above section for these cases, we obtain the following results.

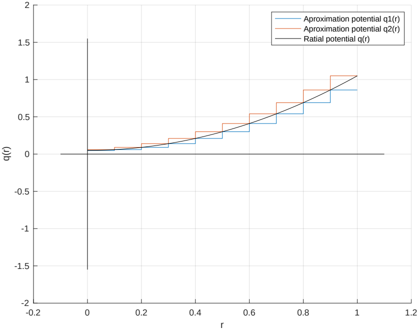

FIGURE – Continuous radial potential in Case 3

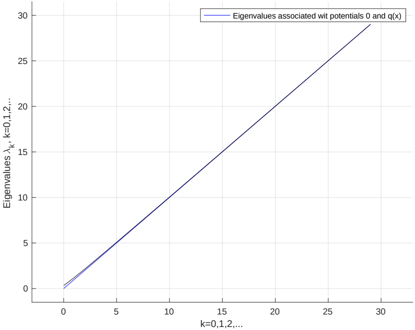

FIGURE – Eigenvalues associated with Continuous radial potential in Case 3

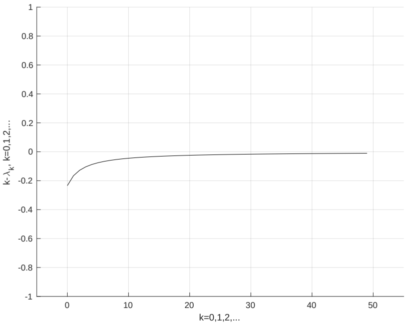

FIGURE – (Eigenvalues-order)-limit in Case 3

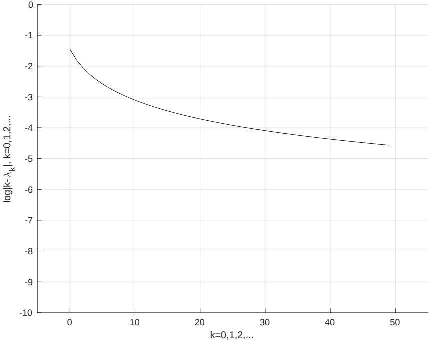

FIGURE – Confirmation eigenvalues limit in Case 3

In Figure 9 we have the potential curve $q(r) = 0.05 + r^2$ in red and this with its approximation by a piecewise constant radial potential in black.
In Figure 10 we see the corresponding eigenvalues. As excepted, we confirm in 11 and 12. These figures show that the eigenvalues defining the Dirichlet-to-Neuman map in theorem (4.2) verify the 1 to 3 properties considered in **Section 2**.

Remark

Theorems are essential tools to determine the explicit expression of the DN map when f, defined in $\mathbb{S}^2$, is usually written as Fourier series $f(\theta) = \sum_{\ell=0}^{\infty} \sum_{k=-\ell}^{\ell} \widehat{f_{\ell k}} Y_\ell^k(\theta)$.

These results are very important for studying the inverse problem for our Schrödinger equation.
We are interesting by the stability of the map that associates a Dirichlet-to-Neumann map to any potential.
That is the purpose of the following section.

Outline

In this section, we are interested by the map

$$\begin{array}{rcl} \Lambda : L^\infty(\mathbb{S}^2) \to \mathcal{L}(H^{1/2}(\mathbb{S}^2), H^{-1/2}(\mathbb{S}^2)) \\ q \quad \longmapsto \quad \Lambda_q, \end{array} \tag{14}$$

where the Dirichlet-to-Neumann map Λ_q is defined in theorem (4.1).
This is an important role in the inverse potential problem, which consists to study its inversion.
In the mathematical literature, the Dirichlet to Neumann map is invertible on its range.

Take into account how the measurements for the inverse problem for our Schrödinger equation are made at the $\mathbb{S}^2$, we know that there may be some noise in the measured Dirichlet-to-Neumann map and that the noisy version of the real Dirichlet-to-Neumann map may not be a Dirichlet-to-Neumann map corresponding to piecewise constant potentials.
Therefore, the stability analysis of Λ, possibly including a regularization strategy useful for the numerical algorithm, would be interesting.

We are interested in a quantification of the difference of two potentials in the L^∞ topology in terms of the distance of their associated Dirichlet-to-Neumann maps.
This stability is necessary for all reconstruction algorithms to recover the potential from the Dirichlet-to-Neumann map.
Then we would like to estimate $q_1 - q_2$ in a certain norm defined by

$$\|\Lambda_{q_1} - \Lambda_{q_2}\|_{H^{1/2} \longrightarrow H^{-1/2}} = \sup_{f \in H^{1/2}(\mathbb{S}^2), f \neq 0} \frac{\|(\Lambda_{q_1} - \Lambda_{q_2})f\|_{H^{-1/2}(\mathbb{S}^2)}}{\|f\|_{H^{1/2}(\mathbb{S}^2)}}$$

There are stability results when the potential q has some smoothness.

We work in the case of piecewise constant arbitrary potentials q. Let us introduce for $n \geq 1$and finite, $m = 1, 2, ..., n$ and $0 = r_0 < r_1 < \cdots < r_{n-1} < r_n = 1$, the space

$$\mathcal{Q} = \left\{ q \in \mathrm{L}^{\infty}(B) : q(r) = \sum_{m=1}^{n} \gamma_m \chi_{(r_{m-1}, r_m)}, \right\}$$

$$r = |x|, r_m \in [0, 1], \gamma_m \in \mathbb{R}$$

In the case where $\gamma_m = 0, m = 1, 2, ..., n$, we approximate it by -0.01.

Here, we establish Lipschitz stability by giving a constant, which depends on n and ℓ in the dimension n of the potential space.

Theorem

Let the unit ball B in $\mathbb{R}^3$ *and the scaled potential* $q_i, i = 1, 2$ *verifes*

$$q_i(r) = \sum_{m=1}^{n} \gamma_m^i \chi_{(r_{m-1}, r_m)}, i = 1, 2, r = |x|,$$

Where $n \geq 1, \gamma_m^i,\ r_m \in \mathbb{R}$, *with* $m = 1, 2, ..., n$ *and* $0 = r_0 < r_1 < \cdots < r_{n-1} < r_n = 1$, *and* $k_m^i = \sqrt{|\gamma_m^i|}$, *such that the Dirichlet problems for* $-\Delta + q_i$ *is well-posed.*

Assume that $\gamma_n^1 \times \gamma_n^2 > 0$ and there is a positive constant M such that

$$\|q_i\|_{L^\infty(B)} \leq M.$$

Then there is a constant $C = C(n, M, \ell)$, such that :

$$|\gamma_n^1 - \gamma_n^2| \leq C(\|\Lambda_{q_1} - \Lambda_{q_2}\|_{H^{1/2} \longrightarrow H^{-1/2}}). \tag{15}$$

The result gives us the Lipschitz stability near to the edge $\mathbb{S}^2$.

For the proof, we consider $q_i \in \mathcal{Q}, i = 1, 2$, and write

$$q_1(r) = \sum_{m=1}^{n} \gamma_m^1 \chi_{(r_{m-1}^1, r_m^1)} \text{ and}$$

$$q_2(r) = \sum_{m=1}^{n} \gamma_m^2 \chi_{(r_{m-1}^2, r_m^2)}, r = |x|,$$

for $n \geq 1, m = 1, 2, ..., n, \gamma_m^1, r_m^1, \gamma_m^2, r_m^2 \in \mathbb{R}$,
$0 = r_0^1 < r_1^1 < \cdots < r_{n-1}^1 < r_n^1 = 1$ and
$0 = r_0^2 < r_1^2 < \cdots < r_{n-1}^2 < r_n^2 = 1$. We assume that
$r_m^1 = r_m^2 = r_m$ for all $m = 0, 1, 2, ...$. Then, we apply results from theorem (4.1).

Remark

The study of stability for a continuous radial potential function would follow from the study of stability in the case where the potential is a piecewise radial function. It is sufficient to approximate this continuous function by two piecewise radial functions.

Outline

Conclusion

- We determine the explicit formula for the Dirichlet-to-Neumann map for all piecewise constant radial potential function and for all continuous radial potential function,
- We also numerically prove the validity of the results.
- We establish a Lipschitz stability result near the edge of the domain with a constant depending on the dimension of the potential space and the order of the eigenvalues

Perspectives

- In future works, it would be interesting to study of the Dirichlet to Neumann map in the case where the potential has one or more zeros on the interval $(0,1)$.
- And, a Lipschitz type stability in the depth of the domain by giving an estimation constant.

Bibliography

1. Calderón A. P., *On an inverse boundary value problem*, Seminar on Numerical Analysis and its Applications to Continuum Physics (Río de Janeiro, 1980), pp. 65-73, Soc. Brasil. Mat., Río de Janeiro, 1980.
2. Calderón A. P., *Boundary value problems for elliptic equations. Outlines of the joint Soviet-American symposium on partial differential equations*, Novisibirsk (1963), 303-304.
3. Fagueye N., *Explicit formula for the Dirichlet to Neumann map for radial potential in dimension 3,*, Journal of Applied Mathematics and Physics (JAMP),

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