

THE UNIQUENESS THEOREM FOR HYDROGEN ATOM EQUATION

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ABSTRACT. In this article, we prove that the difference between two potential functions becomes sufficiently small whenever the spectrums are chosen sufficiently close to each other.

Keywords: Sturm-Liouville problem, spectrum, asymptotic formula, norming constants, hydrogen atom.

AMS Subject Classification: 31A25, 31B20.

1. INTRODUCTION

The importance of mathematics arises from the study of problems in the real world. Inverse problem for the differential operator consists of reconstruction of the operator by its spectral data. The spectral characteristics are spectra, spectral functions, scattering data, norming constants, etc. The concept of inverse problem plays an important role in mathematics and physics. The progress in applied mathematics has been obtained by the extension and development of many important analytical approaches and methods.

Borg [3] proved that two spectra uniquely determine the potential of the Sturm-Liouville equation. Tikhonov [18] proved uniqueness of the solution of the problem of electromagnetic sounding. Marchenko [13, 14] showed that two various spectra of the one singular Sturm-Liouville equation determine this equation uniquely. Later, Krein [10] gave solution of the inverse Sturm-Liouville problem. Gelfand -Levitan [5, 6] showed an algorithm for construction of $q(x); h$ and H . Also inverse problems for singular equations have been shown in the monographs in [4, 9]. Further Mizutani [15] improved a different algorithm, which is a slight modification of Gelfand-Levitan's model. One of this kind of inverse problems was considered by numerous authors (see [1], [2], [7-9], [12], [16], [17]).

In this paper, we consider singular Sturm-Liouville equation:

$$\frac{d^2 R}{dr^2} + \frac{a}{r} \frac{dR}{dr} - \frac{\ell(\ell+1)}{r^2} R + \left(E + \frac{a}{r}\right) R = 0 \quad (0 < r < \infty). \quad (1)$$

In quantum mechanics the study of the energy levels of the hydrogen atom leads to this equation [12]. Here R is the distance of the mass center to the origin, ℓ is a positive integer, a is a real number, E is an energy constant and r is the distance between the nucleus and electron.

In [15] Mizutani showed the uniqueness of the potential function for regular Sturm-Liouville problem according to normalizing constants and eigenvalues. Our aim is to apply the same method for singular Sturm-Liouville problem.

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2. PRELIMINARY KNOWLEDGE

Substitution $R = y/r$ reduces equation (1) to the form

$$\frac{d^2 y}{dr^2} + \left\{ E + \frac{a}{r} - \frac{\ell(\ell+1)}{r^2} \right\} y = 0. \quad (2)$$

In most cases we took the reference potential to be

$$V(r) = \frac{a}{r} - \frac{\ell(\ell+1)}{r^2}.$$

When $V(r)$ is defined by last differential equation, it contains a centripetal and Colomb part, the usual singularities of the nuclear problem [2].

Just as in the case of Bessel's equation, one can show that in a finite interval $[0, b]$, the spectrum is discrete. From [12] and [1], the solution of (2) is bounded at zero.

Now, consider $\{\lambda_n\}_{n=0}^{\infty}$ as a spectrum of the following singular Sturm-Liouville problem

$$Ly = -y'' + q(r)y = \lambda y, \quad (0 < r \leq \pi) \quad (3)$$

with boundary conditions

$$y(0) = 0, \quad (4)$$

$$y(\pi, \lambda) \cos \beta + y'(\pi, \lambda) \sin \beta = 0, \quad (5)$$

where $q(r) = \frac{\ell(\ell+1)}{r^2} - \frac{a}{r} + q_0(r)$ and β is a real number.

Consider Sturm-Liouville equation for having different potential

$$\tilde{L}y = -y'' + \tilde{q}(r)y = \tilde{\lambda}y, \quad (0 < r \leq \pi), \quad (6)$$

where $\tilde{q}(r) = \frac{\ell(\ell+1)}{r^2} - \frac{\tilde{a}}{r} + \tilde{q}_0(r)$.

Let $\{\tilde{\lambda}_n\}_{n=0}^{\infty}$ be the spectrum of (6) with (4)-(5).

One has the following asymptotic formulas for solutions $\varphi(r, \lambda)$, of the problem (3),(4) eigenvalues λ_n , $\tilde{\lambda}_n$ and normalizing coefficients α_n , $\tilde{\alpha}_n$, respectively (see [1, 2])

$$\varphi(r, \lambda) = \cos \left[(n + \ell/2)r - \frac{\ell\pi}{2} \right] + O\left(\frac{\ln n}{n}\right), \quad (7)$$

$$\varphi'(r, \lambda) = -(n + \ell/2) \sin \left[(n + \ell/2)r - \frac{\ell\pi}{2} \right] + O\left(\frac{\ln n}{n}\right). \quad (8)$$

$$\lambda_n = \left(n + \frac{\ell}{2}\right)^2 + \frac{a}{\pi} \ln \left(n + \frac{1}{2}\right) + O\left(\frac{\ln^2 n}{n^3}\right), \quad (9)$$

$$\tilde{\lambda}_n = \left(n + \frac{\ell}{2}\right)^2 + \frac{\tilde{a}}{\pi} \ln \left(n + \frac{1}{2}\right) + O\left(\frac{\ln^2 n}{n^3}\right).$$

$$\alpha_n = \|\varphi_n\|^2 = \int_0^\pi \varphi_n^2(r) dr = \frac{\pi}{2} + \frac{a\pi^2}{4} \frac{1}{n + \frac{1}{2}} + O\left(\frac{\ln n}{n^3}\right), \quad (10)$$

$$\tilde{\alpha}_n = \|\tilde{\varphi}_n\|^2 = \int_0^\pi \tilde{\varphi}_n^2(r) dr = \frac{\pi}{2} + \frac{\tilde{a}\pi^2}{4} \frac{1}{n + \frac{1}{2}} + O\left(\frac{\ln n}{n^3}\right). \quad (11)$$

Theorem 2.1 (17). *Let D be a linear topological space and $D_1, D_2 \subset D$. The transformation operator, $X = X_{L, \tilde{L}}$, mapping D_1 to D_2 can be defined as follows*

$$X[\varphi(r, \lambda)] = \tilde{\varphi}(r, \lambda) = \varphi(r, \lambda) + \int_0^r K(r, s) \varphi(s, \lambda) ds. \tag{12}$$

The kernel in operator (12) is a solution of the differential equation

$$\frac{\partial^2 K(r, s)}{\partial r^2} - \left(\frac{\ell(\ell+1)}{r^2} - \frac{\tilde{a}}{r} + \tilde{q}_0(r) \right) K(r, s) = \frac{\partial^2 K(r, s)}{\partial s^2} - \left(\frac{\ell(\ell+1)}{s^2} - \frac{a}{s} + q_0(s) \right) K(r, s)$$

and also satisfies the following conditions

$$K(r, r) = \frac{1}{2} \int_0^r (\tilde{q}(s) - q(s)) ds, \tag{13}$$

$$K(r, 0) = 0.$$

Lemma 2.1. *There exists a constant $M > 0$, such that*

$$|\varphi(r, \lambda)| + \frac{|\varphi'(r, \lambda)|}{\lambda} \leq M, \tag{14}$$

$$\lambda \left| \dot{\varphi}(r, \lambda) \right| + \left| \dot{\varphi}'(r, \lambda) \right| \leq M \tag{15}$$

hold for every $\lambda \geq 1$ and $0 < r \leq \pi$ ($\dot{\varphi}(r, \lambda) = \frac{d\varphi}{d\lambda}$).

Proof. Using the equations (7) and (8) in (14), we obtain the following inequality

$$\left[\left| \cos \left[(n + \ell/2)r - \frac{\ell\pi}{2} \right] \right| + \frac{\left| - (n + \ell/2) \sin \left[(n + \ell/2)r - \frac{\ell\pi}{2} \right] + O\left(\frac{\ln n}{n}\right) \right|}{\lambda_n} \right] \leq M,$$

where $0 < r \leq \pi$ and $-1 \leq \cos \left[(n + \ell/2)r - \frac{\ell\pi}{2} \right] \leq 1$, $-1 \leq \sin \left[(n + \ell/2)r - \frac{\ell\pi}{2} \right] \leq 1$. Then using the formulas (9), we obtain (14). We can find inequality (15), in a similar way. \square

Note that using

$$F(r, s) = \sum_{n=1}^{\infty} \left[\frac{\varphi(r, \tilde{\lambda}_n) \varphi(s, \tilde{\lambda}_n)}{\tilde{\alpha}_n} - \frac{\varphi(r, \lambda_n) \varphi(s, \lambda_n)}{\alpha_n} \right] \tag{16}$$

we have

$$K(r, s) + F(x, s) + \int_0^r K(r, t) F(t, s) dt = 0 \quad \text{for } 0 < s \leq r \leq \pi.$$

In [15] Mizutani showed the uniqueness of the potential function for Sturm-Liouville problem according to normalizing constants and eigenvalues. The purpose of our study is to give the scture concerning the difference $q(r) - \tilde{q}(r)$ for the differential operators having the singularity type $\frac{\ell(\ell+1)}{r^2} - \frac{a}{r}$, by using Mizutani method.

3. MAIN RESULTS

Main result of the paper is given by the following theorem.

Theorem 3.1. *If*

$$\mathbf{A} \equiv \sum_{n=1}^{\infty} \left[|\tilde{\alpha}_n - \alpha_n| + \left| \tilde{\lambda}_n - \lambda_n \right| \right] \quad (17)$$

is sufficiently small, then we get

$$\max_{0 < r \leq \pi} |q(r) - \tilde{q}(r)| \leq C_1 A, \quad (18)$$

where $C_1 > 0$ is a constant depending only on $q(r)$ and h .

Proof. Let's solve the linear integral equation (16). Firstly let us start from $F(s, t)$, then constructing the iterated kernels $F^{(n)}(s, t; r)$, ($n = 1, 2, \dots$). We get,

$$F^{(1)}(s, t; r) = F(s, t), \quad F^{(n+1)}(s, t; r) = \int_0^r F(s, u) F^{(n)}(u, t; r) du, \quad n \geq 1. \quad (19)$$

We take

$$S(s, t; r) = \sum_{n=1}^{\infty} (-1)^n F^{(n)}(s, t; r),$$

furthermore, assuming that

$$\int_0^r \int_0^r |F(s, t)|^2 ds dt < 1 \quad (20)$$

we can see that

$$K(r, s) = S(r, s; r) \quad (21)$$

for $0 < s \leq r \leq \pi$.

Then it follows from (13) that

$$\frac{1}{2}(q(r) - \tilde{q}(r)) = -\frac{d}{dr}K(r, r). \quad (22)$$

Let's give the following Lemma and its proof to complete the proof of the Theorem 3.1.

Lemma 3.1. *By virtue of the (16), let us define $F(r, s)$. Then we get*

$$\frac{1}{2}(q(r) - \tilde{q}(r)) = -\frac{d}{dr}F(r, r) - K^2(r, r) + 2 \int_0^r F_r(r, u) K(r, u) du,$$

where $F(r, s)$ has a continuous derivative and the condition (20) is satisfied.

Proof. Using formula (19)-(22), we obtain the following equation

$$\frac{1}{2}(q(r) - \tilde{q}(r)) = \frac{d}{dr}F(r, r) + \sum_{n=1}^{\infty} (-1)^n \frac{d}{dr}F^{(n+1)}(r, r; r). \quad (23)$$

Now we estimate $\frac{d}{dr}F^{(n+1)}(r, r; r)$:

$$\begin{aligned} \frac{d}{dr}F^{(n+1)}(r, r; r) &= \left\{ F_s^{(n+1)} + F_t^{(n+1)} + F_r^{(n+1)} \right\}_{\substack{s=r \\ t=r}} = \\ &= \left\{ \int_0^r F_s(s, u) F^{(n)}(u, t; r) du + \int_0^r F^{(n)}(s, u; r) F_t(u, t) du + F^{(n+1)} \right\}_{\substack{s=r \\ t=r}} = \\ &= 2 \int_0^r F_r(r, u) F^{(n)}(r, u; r) du + \frac{\partial}{\partial r} \left(\int_0^r F(s, u) F^{(n)}(u, t; r) du \right)_{\substack{s=r \\ t=r}} = \\ &= 2 \int_0^r F_r(r, u) F^{(n)}(r, u; r) du + \sum_{k=1}^n F^{(k)}(r, r; r) F^{(n+1-k)}(r, r; r). \end{aligned} \quad (24)$$

Using (24) in (23), the equation

$$\frac{1}{2}(q(r) - \tilde{q}(r)) = \frac{d}{dr}F(r, r) + 2 \int_0^r F_r(r, u) K(r, u) du - K^2(r, r)$$

is obtained. □

Now, we can prove the of Theorem 3. Let us take A_0 as follows:

$$A_0 = \frac{1}{2} \inf_n \alpha_n.$$

A_0 is positive from the asymptotic formula (9), (10) and (11). We suppose that

$$A \equiv \sum_{n=0}^{\infty} \left[|\tilde{\alpha}_n - \alpha_n| + |\tilde{\lambda}_n - \lambda_n| \right] \leq A_0. \quad (25)$$

Then we get

$$\alpha_n \geq 2A_0 \quad \text{and} \quad \tilde{\alpha}_n \geq A_0 \quad \text{for each } n. \quad (26)$$

Differentiating formally the right side of (16) with respect to r , we obtain the following equation

$$F_r(r, s) = \sum_{n=1}^{\infty} \left[\frac{\varphi'(r, \tilde{\lambda}_n) \varphi(s, \tilde{\lambda}_n)}{\tilde{\alpha}_n} - \frac{\varphi'(r, \lambda_n) \varphi(s, \lambda_n)}{\alpha_n} \right].$$

Let's add $\frac{\varphi'(r, \lambda_n) \varphi(s, \lambda_n)}{\tilde{\alpha}_n}$ to last equation and then subtract it. Then we find

$$F_r(r, s) = \sum_{n=1}^{\infty} \left[\left(\frac{\alpha_n - \tilde{\alpha}_n}{\tilde{\alpha}_n \alpha_n} \right) \varphi'(r, \lambda_n) \varphi(s, \lambda_n) + \frac{1}{\tilde{\alpha}_n} \int_{\lambda_n}^{\tilde{\lambda}_n} (\varphi'(r, \lambda) \varphi(s, \lambda))' d\lambda \right].$$

By virtue of (25) and (26) and Lemma 1 it is seen that $F(r, s)$ has a continuous derivative and

$$|F_r(r, s)| \leq C' \sum_{n=1}^{\infty} \left[|\tilde{\alpha}_n - \alpha_n| + |\tilde{\lambda}_n - \lambda_n| \right] \equiv C' A. \quad (27)$$

We can also write

$$\left| \frac{d}{dr} F(r, r) \right| \leq 2C' A.$$

Using the same method, we obtain

$$\begin{aligned} |F(r, s)| &= \sum_{n=1}^{\infty} \left| \left(\frac{\alpha_n - \tilde{\alpha}_n}{\tilde{\alpha}_n \alpha_n} \right) \varphi(r, \lambda_n) \varphi(s, \lambda_n) + \frac{1}{\tilde{\alpha}_n} \int_{\lambda_n}^{\tilde{\lambda}_n} [\varphi(r, \lambda) \varphi(s, \lambda)] d\lambda \right| \\ |F(r, r)| &= \sum_{n=1}^{\infty} \left| \left(\frac{\alpha_n - \tilde{\alpha}_n}{\tilde{\alpha}_n \alpha_n} \right) \varphi(r, \lambda_n)^2 + \frac{1}{\tilde{\alpha}_n} \int_{\lambda_n}^{\tilde{\lambda}_n} [2\dot{\varphi}(r, \lambda) \varphi(r, \lambda)] d\lambda \right|. \end{aligned}$$

By means of asymptotic formulas (7), (8) and $0 < r \leq \pi$, $-1 \leq \sin r \leq 1$, $-1 \leq \cos r \leq 1$,

$$\begin{aligned} |F(r, r)| &= \sum_{n=1}^{\infty} \left| \left(\frac{\alpha_n - \tilde{\alpha}_n}{\tilde{\alpha}_n \alpha_n} \right) \left(\cos \left[(n + \ell/2) r - \frac{\ell\pi}{2} \right] + O \left(\frac{\ln n}{n} \right) \right)^2 - \right. \\ &\quad \left. - \frac{1}{\tilde{\alpha}_n} \int_{\lambda_n}^{\tilde{\lambda}_n} 2 \left[\sqrt{\lambda} \sin \left[(\sqrt{\lambda}) r - \frac{\ell\pi}{2} \right] + O \left(\frac{\ln n}{n} \right) \right] \times \right. \\ &\quad \left. \times \left[\left(\cos \left[(n + \ell/2) r - \frac{\ell\pi}{2} \right] + O \left(\frac{\ln n}{n} \right) \right) \right] d\lambda \right|. \end{aligned}$$

It follows from the last equation that

$$\begin{aligned} |F(r, r)| &\leq \sum_{n=1}^{\infty} \left| \left(\frac{\alpha_n - \tilde{\alpha}_n}{\tilde{\alpha}_n \alpha_n} \right) c_1 - \frac{1}{\tilde{\alpha}_n} \int_{\lambda_n}^{\tilde{\lambda}_n} 2c_2 d\lambda \right| = \\ &= C'' \sum_{n=1}^{\infty} |\tilde{\alpha}_n - \alpha_n| + |\tilde{\lambda}_n - \lambda_n|. \end{aligned} \tag{28}$$

From (28), we estimate

$$|F(r, r)| \leq C'' A,$$

where C' and C'' are constants depending only on $q(x)$ and h .

If $\pi C'' A$ is sufficiently small e.g., $\pi C'' A < \frac{1}{2}$, using formula (21), we can write the following equation

$$|K(r, s)| = \sum_{n=1}^{\infty} (-1)^n F^{(n)}(r, s; r). \tag{29}$$

Because of formula (19), we construct the iterated kernels $F^{(n)}$ as follows:

$$\begin{aligned} |F^{(1)}| &= |F(r, r)| \leq C'' A, \\ |F^{(2)}| &= \left| \int_0^r F F^{(1)} du \right| = \left| \int_0^r F F du \right| \leq \left| \int_0^r (C'' A)^2 du \right| = (C'' A)^2 \pi \\ |F^{(3)}| &= \left| \int_0^r F F^{(2)} du \right| = \left| \int_0^r (C'' A) (C'' A)^2 \pi du \right| \leq \left| \int_0^r (C'' A)^3 \pi^2 du \right| = (C'' A)^3 \pi^2 \end{aligned}$$

$$\begin{aligned} & \vdots \\ |F^{(n)}| & \leq \frac{1}{\pi} (\pi C'' A)^n. \end{aligned} \quad (30)$$

Using (29) in (28), we get

$$|K(r, s)| \leq \left| \sum_{n=1}^{\infty} \frac{1}{\pi} (\pi C'' A)^n \right| \leq 2C'' A. \quad (31)$$

By Lemma 2 and (27)-(31), consequently, we obtain

$$|q(r) - \tilde{q}(r)| \leq C_1 \sum_{n=1}^{\infty} \left[|\tilde{\alpha}_n - \alpha_n| + |\tilde{\lambda}_n - \lambda_n| \right]$$

for $A \leq \min \left\{ A_0, (2\pi C'')^{-1} \right\}$. This completes the proof. \square

We can give the following numerical example as an application of Theorem 3.1.

Example. If we substitute $a = \frac{1}{4}$, $\ell = 1$, $q_0(r) = 0$ and $\tilde{a} = \frac{1}{6}$, $\ell = 1$, $\tilde{q}_0(r) = 0$ in to the equations (3) and (6) respectively, then we obtain the following equations

$$-y'' + \left(\frac{2}{r^2} - \frac{1}{4r} \right) y = \lambda y \quad (32)$$

and

$$-y'' + \left(\frac{2}{r^2} - \frac{1}{6r} \right) y = \lambda y. \quad (33)$$

According to the equations (32) and (33) we can write the formulas (9), (10) and (11) in the following forms respectively. For $n = 1$,

$$\begin{aligned} \alpha_1 &= \frac{\pi}{2} + \frac{\pi^2}{24}, & \lambda_1 &= \frac{9}{4} + \frac{\ln \frac{3}{2}}{4\pi}, \\ \tilde{\alpha}_1 &= \frac{\pi}{2} + \frac{\pi^2}{36}, & \tilde{\lambda}_1 &= \frac{9}{4} + \frac{\ln \frac{3}{2}}{6\pi}. \end{aligned}$$

Taking $h = 1$, $r = 0, 1$, $\pi \approx 3$, $\ln \frac{3}{2} \approx 0, 4$, we get,

$$A \approx 0, 13611.$$

Choosing $C_1 = \frac{q(r)}{30h}$ we have

$$C_1 A \approx 0, 89606.$$

According to the given data, difference of the potential functions is 0,83333 approximately. Therefore inequality (18) is satisfied.

Let the spectral datas of the first equation be the same and change normalizing coefficients and eigenvalues of the second equation as follows:

$$\tilde{\alpha}_1 = \frac{\pi}{2} + \frac{\pi^2}{30}, \quad \tilde{\lambda}_1 = \frac{9}{4} + \frac{\ln \frac{3}{2}}{5\pi}.$$

By necessary computations, we find that

$$C_1 A \approx 0, 53763$$

$$\max_{0 < r \leq \pi} |q(r) - \tilde{q}(r)| = 0, 5$$

where $\tilde{a} = \frac{1}{5}$.

Similarly, taking $\tilde{a} = 0, 26$ we obtain the following equations

$$\tilde{\alpha}_1 = \frac{\pi}{2} + \frac{26\pi^2}{600}, \quad \tilde{\lambda}_1 = \frac{9}{4} + \frac{26}{300} \ln \frac{3}{2},$$

$$C_1 A \cong 0, 105,$$

$$\max_{0 < r \leq \pi} |q(r) - \tilde{q}(r)| = 0, 1.$$

As we can see from the discussions above, if the normalizing coefficients and eigenvalues are chosen very close to each other, then the difference of potential functions becomes sufficiently small.

Obviously, we see that Theorem 3.1 is satisfied by example.

4. CONCLUSION

In this paper, we have extended the scope of the Mizutani method by proving the uniqueness theorem for the differential operator having the singularity type $\frac{\ell(\ell+1)}{r^2} - \frac{a}{r}$.

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