A Practical Method for Solving the Inverse Quantum Scattering Problem on a Half Line

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Abstract. A method for solving inverse quantum scattering problems on a half line is proposed. It is based on the application of the transmutation operators and recent results on series expansion of the integral transmutation kernels. From the corresponding Gel'fand-Levitan equation a system of linear algebraic equations is derived for the coefficients of the Fourier-Legendre series expansion of the output (transmutation operator) kernel. It is shown that the knowledge of the very first coefficient is sufficient for recovering the potential and hence for solving the inverse problem. A numerical illustration is presented.

1. Introduction

A direct and practical method is presented for solving the classical inverse quantum scattering problem on the half-line. It is based on the ideas developed in [1], [2], [3] and allows one to reduce the inverse scattering problem directly to a system of linear algebraic equations from which the first component of the solution vector is sufficient for recovering the potential. To obtain the system of equations the Fourier-Legendre series representation for the output kernel (the kernel of a transmutation operator) from [4] is used together with the Gel'fand-Levitan equation. The Fourier-Legendre coefficients satisfy a system of linear algebraic equations derived from the Gel'fand-Levitan equation, and a crucial fact is that the knowledge of the very first coefficient allows one to recover the potential. In practical terms this means that a reduced number of equations in the truncated system of equations is already sufficient to obtain the recovered potential with a remarkable accuracy. Thus, the method proposed possesses the following advantageous features. It is direct (not iterative as existing competitive methods for solving inverse spectral problems, e.g., [5]), simple (its numerical implementation is an easy task) and fast (no more than several seconds were needed to perform the computation presented on a laptop equipped with an Intel (R) Core (TM) Processor @ 0.80 GHZ 998 MHz).
2. Preliminaries on scattering data and useful relations

Consider the one-dimensional Schrödinger equation

\[-y'' + q(x)y = \lambda y, \quad x > 0,\]  

with \(q(x)\) being a real valued short range potential, that is, a real valued integrable function satisfying the condition

\[\int_0^\infty (1 + |x|)|q(x)|dx < \infty.\]  

The square root of the spectral parameter \(\lambda \in \mathbb{C}\) we denote by \(\rho\), \(\lambda = \rho^2\) and choose it such that \(\tau := \text{Im} \rho \geq 0\). Denote \(\Omega_+ := \{\rho : \tau > 0\}\).

Denote by \(\psi(\rho, x)\) a solution of (1) satisfying the initial conditions

\[\psi(\rho, 0) = 0, \quad \psi'(\rho, 0) = 1.\]  

It admits the following Povzner-Levitan representation

\[\psi(\rho, x) = \frac{\sin \rho x}{\rho} + \int_0^x S(x, t) \frac{\sin \rho t}{\rho} dt,\]  

where

\[S(x, t) = -\frac{1}{\pi} \int_0^\infty \left( \psi(\rho, x) - \frac{\sin \rho x}{\rho} \right) \sin \rho t d\rho,\]  

\(S(x, 0) = 0, S(x, x) = \frac{1}{2} \int_0^x q(t)dt[6].\)

It is well known (see, e.g., [7], [8, Theorem 2.4.1]) that (1) possesses the unique so-called Jost solution \(y = e(\rho, x)\) such that for \(\nu = 0, 1\), the asymptotic relation

\[e^{(\nu)}(\rho, x) = (i\rho)^\nu e^{i\rho x} (1 + o(1)), \quad x \to \infty\]  

holds uniformly in \(\Omega_+\). For every \(\rho \in \Omega_+\) the function \(e(\rho, x)\) belongs to \(L_2(0, \infty)\). The following asymptotic relation for large values of \(|\rho|\),

\[e^{(\nu)}(\rho, x) = (i\rho)^\nu e^{i\rho x} \left( 1 + \frac{\omega(x)}{\rho} + o \left( \frac{1}{\rho} \right) \right), \quad |\rho| \to \infty,\]  

\[\omega(x) := -\frac{1}{2} \int_x^\infty q(t)dt,\]

is valid uniformly with respect to \(x \geq 0\) [8, p. 129].

The function \(e(\rho, x)\) admits the following representation

\[e(\rho, x) = e^{i\rho x} + \int_x^\infty A(x, t) e^{i\rho t} dt,\]  

where \(A\) is a real valued function such that

\[A(x, x) = \frac{1}{2} \int_x^\infty q(t)dt,\]  

with \(A(x, \cdot) \in L_2(x, \infty)\). Formula (6) is called Levin’s representation of the Jost solution (see, e.g., [6, Ch. 5, Sect. 1]). In [9] a new series representation was derived for \(e(\rho, x)\) based on (6).
Note that the potential $q$ can be recovered from any of the kernels $S(x,t)$ or $A(x,t)$ as

$$q(x) = 2 \frac{d}{dx} S(x,x) = -2 \frac{d}{dx} A(x,x).$$

The function $F(\rho) := e(\rho, 0)$ is called the \textit{Jost function} and the quotient

$$S(\rho) := \frac{F(-\rho)}{F(\rho)}$$

is traditionally called the scattering or simply $S$-matrix. Notice that due to (5) we have that

$$F(\rho) = 1 + \frac{\omega(x)}{i\rho} + o\left(\frac{1}{\rho}\right), \quad |\rho| \to \infty. \quad (9)$$

The potential $q$ may admit a finite number of bound states, the physical solutions square integrable on $(0, \infty)$. They may exist for certain negative values of the parameter $\lambda$ called eigenvalues. Usually, the set of the scattering data is introduced as follows

$$\left\{ S(\rho), \rho > 0; \left\{\rho_j^2, s_j\right\}_{j=1}^N \right\}$$

where $\rho_j^2$ are the eigenvalues and $s_j$ are the corresponding norming constants [10],

$$s_j := \frac{1}{\int_0^\infty e^2(\rho_j, x)dx} = -\frac{2\rho_j}{F(\rho_j)e'(\rho_j, 0)}, \quad (10)$$

where $\dot{F}$ means the derivative with respect to $\rho$. The forward scattering problem consists in finding the scattering data, given a potential $q$ satisfying (2), and the inverse scattering problem requires finding $q$, given the scattering data.

Solution of the forward scattering problem reduces in fact to finding the Jost solution and its derivative. Then the eigenvalues (if exist) correspond to zeros of the Jost function $F(\rho)$, $\text{Im} \rho \geq 0$. The norming constants are computed by (10), and $S(\rho)$ is obtained from (8).

The inverse problem can be solved via the Marchenko equation (see, e.g., [6, Chapter V])

$$A(x, y) = A_0(x + y) + \int_x^\infty A(x, s) A_0(s + y)ds, \quad y > x, \quad (11)$$

where the kernel $A_0$ is constructed from the scattering data,

$$A_0(y) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} (S(\rho) - 1) e^{i\rho y} d\rho + \sum_j s_j e^{i\rho_j y} \quad (12)$$

or via the Gel’fand-Levitan equation (see, e.g., [6, Chapter III])

$$S(x, y) + F(x, y) + \int_0^x S(x, s) F(s, y)ds = 0, \quad (13)$$

where

$$F(x, y) = \frac{2}{\pi} \int_0^\infty \sin \rho x \sin \rho y \left(\frac{1}{|F(\rho)|^2} - 1\right) d\rho + \sum_j c_j \sinh (i\rho_j x) \sinh (i\rho_j y) \quad (14)$$

and

$$c_j := \frac{1}{\int_0^\infty \psi^2(\rho_j, x)dx} = -\frac{2\rho_j e'(\rho_j, 0)}{F(\rho_j)}. \quad (15)$$
As it is pointed out in [6, p. 73] the approach based on the Marchenko equation for solving the inverse problem is somewhat simpler than the approach based on the Gel’fand-Levitan equation. The reason is that the kernel $A_0$ is obtained directly from the scattering data without the necessity of some extra calculations required for the computation of the Jost function using relations (I.4.11) and (II.2.1) from [6] which represents an additional computational challenge. However, as it is discussed by the physicists involved in numerical solution of the inverse quantum scattering problems (see, e.g., [11]) the Gel’fand-Levitan approach is preferable “since use of the Marchenko set encounters numerical difficulties”.

In the present work we develop a method for solving the inverse problem using as a starting point the Gel’fand-Levitan equation and assume $F(\rho)$ to be given.

3. Series representations for the output kernels

In [4] the following representation for the kernel $S(x, y)$ was obtained

$$S(x, y) = \sum_{n=0}^{\infty} \frac{s_n(x)}{x} P_{2n+1} \left( \frac{y}{x} \right), \quad 0 < y \leq x < \infty,$$  \hspace{1cm} (15)

where $P_m$ stands for a Legendre polynomial of order $m$. For all $x > 0$ the series converges in the norm of $L_2(0, x)$ - space. The coefficients $s_n$ can be computed by a recurrent integration procedure starting with

$$s_0(x) = \frac{3}{2} \left( \frac{\psi(0, x)}{x} - 1 \right).$$  \hspace{1cm} (16)

It is worth mentioning that the knowledge of the procedure is superfluous for the method proposed in the present paper. Only (15) and (16) are required. Notice that equality (16) indicates that the first coefficient $s_0$ is sufficient for recovering the potential $q$. Indeed, since $\psi''(0, x) = q(x)\psi(0, x)$ we have that

$$q(x) = \frac{(xs_0(x))''}{(xs_0(x) + \frac{3}{2}x)}.$$  \hspace{1cm} (17)

4. Linear system of equations for the coefficients $s_n$

In this section we derive a system of linear algebraic equations for the coefficients $\{s_n\}_{n=0}^{\infty}$ from which we are interested in computing the very first coefficient $s_0$.

**Theorem 1** The coefficients of (15) satisfy the system of equations

$$\frac{s_m(x)}{4m + 3} + \sum_{n=0}^{\infty} s_n(x) B_{m,n}(x) = -f_m(x, x), \quad \text{for all } m = 0, 1, \ldots,$$  \hspace{1cm} (18)

where

$$B_{m,n}(x) := (-1)^{n+m} \frac{2x}{\pi} \int_{0}^{\infty} j_{2m+1}(\rho x) j_{2m+1}(\rho x) \left( \frac{1}{|F(\rho)|^2} - 1 \right) \frac{d\rho}{\rho^2}$$

$$+ (-1)^{n+m} i x \sum_{j} c_j j_{2m+1}(\rho_j x) j_{2m+1}(\rho_j x),$$

$$f_m(x, y) := (-1)^{m} \frac{2x}{\pi} \int_{0}^{\infty} j_{2m+1}(\rho x) \sin(py) \left( \frac{1}{|F(\rho)|^2} - 1 \right) \frac{d\rho}{\rho^2}$$

$$+ (-1)^{m} i x \sum_{j} c_j j_{2m+1}(\rho_j x) \sinh(i\rho_j y),$$

$$0 < y \leq x < \infty.$$
with $0 < y \leq x < \infty$, and $j_k$ stands for the spherical Bessel function of order $k$.

**Proof.** The proof is similar to that from [3]. Substitution of (15) into the Gel’fand-Levitan equation (13) leads to the equality

$$
\sum_{n=0}^{\infty} \frac{s_n(x)}{x} \left( P_{2n+1} \left( \frac{y}{x} \right) + \int_0^x F(t,y) P_{2n+1} \left( \frac{t}{x} \right) dt \right) = -F(x,y).
$$

(21)

Note that

$$
\int_0^x F(t,y) P_{2n+1} \left( \frac{t}{x} \right) dt = f_n(x,y).
$$

(22)

Indeed, substitution of (14) into this integral leads to the equality

$$
\int_0^x F(t,y) P_{2n+1} \left( \frac{t}{x} \right) dt = 2 \pi \int_0^\infty \sin(\rho y) \left( \frac{1}{|F(\rho)|} - 1 \right) \int_0^x \sin(\rho t) P_{2n+1} \left( \frac{t}{x} \right) dt d\rho
$$

$$
+ \sum_j c_j \sin(i \rho_j y) \int_0^x \sin(i \rho_j t) P_{2n+1} \left( \frac{t}{x} \right) dt,
$$

from which with the aid of [12, formula 2.17.7.1] we obtain (22). Here due to (9) the integral

$$
\int_0^\infty \sin(\rho t) \sin(\rho y) \left( \frac{1}{|F(\rho)|} - 1 \right) d\rho
$$

is absolutely convergent, and hence Foubini’s theorem can be applied for changing the order of integration.

Hence (21) takes the form

$$
\sum_{n=0}^{\infty} \frac{s_n(x)}{x} \left( P_{2n+1} \left( \frac{y}{x} \right) + f_n(x,y) \right) = -F(x,y).
$$

(23)

For all $x > 0$ and $0 < y \leq x$ the series $\sum_{n=0}^{\infty} (s_n(x)/x) f_n(x,y)$ converges since it is the inner product of $S(x, \cdot)$ with $F(\cdot, y)$ in $L^2(0,x)$. Indeed, since the set of the Legendre polynomials $\{P_{2n+1} \left( \frac{t}{x} \right) \}_{n=0}^{\infty}$ is complete and orthogonal in $L^2(0,x)$ together with (15) we have that

$$
F(t,y) = \sum_{n=0}^{\infty} \left( F(\cdot, y), P_{2n+1} \left( \frac{\cdot}{x} \right) \right) \frac{P_{2n+1} \left( \frac{t}{x} \right)}{\|P_{2n+1} \left( \frac{\cdot}{x} \right)\|_{L^2(0,x)}}
$$

$$
= \frac{1}{x} \sum_{n=0}^{\infty} (4n + 3) f_n(x,y) P_{2n+1} \left( \frac{t}{x} \right).
$$

Consequently (due to the general Parseval relation [13, p. 16]),

$$
\langle G(x, \cdot), F(\cdot, y) \rangle_{L^2(0,x)} = \sum_{n=0}^{\infty} \left( G(x, \cdot), \frac{P_{2n+1} \left( \frac{\cdot}{x} \right)}{\|P_{2n+1} \left( \frac{\cdot}{x} \right)\|_{L^2(0,x)}} \right) \left( F(\cdot, y), \frac{P_{2n+1} \left( \frac{\cdot}{x} \right)}{\|P_{2n+1} \left( \frac{\cdot}{x} \right)\|_{L^2(0,x)}} \right)
$$

$$
= \sum_{n=0}^{\infty} \frac{s_n(x)}{x} f_n(x,y).
$$

Now, multiplying (23) by $P_{2m+1} \left( \frac{y}{x} \right)$ and integrating with respect to $y$ leads to the equality

$$
\frac{s_m(x)}{4m+3} + \sum_{n=0}^{\infty} \frac{s_n(x)}{x} \int_0^x P_{2m+1} \left( \frac{y}{x} \right) f_n(x,y) dy = -f_m(x,x),
$$

for all $m = 0, 1, \ldots$. Simple calculation with the aid of [12, formula 2.17.7.1] shows that

$$
\frac{1}{x} \int_0^x P_{2m+1} \left( \frac{y}{x} \right) f_n(x,y) = B_{m,n}(x)
$$

and hence (18) is obtained. For all $x > 0$ the series $\sum_{n=0}^{\infty} s_n(x) B_{m,n}(x)$ converges, again due to the general Parseval equality as the inner product of $S(x, \cdot)$ with $f_m(x, \cdot)$ in $L^2(0,x)$. •
5. Numerical realization and illustration

Theorem 1 together with equality (17) leads to a simple and direct numerical algorithm for solving the inverse quantum scattering problem on a half-line. Given the spectral data,

(i) compute approximations of $f_m(x, x)$ and $B_{m,n}(x)$ by formulas (19) and (20);
(ii) for a set of points $\{x_l\}$ from $(0, b], b > 0$ solve the system

$$\frac{s_m(x)}{4m + 3} + \sum_{n=0}^{M} s_n(x)B_{m,n}(x) = -f_m(x, x), \quad m = 0, 1, \ldots, M, \quad (24)$$

obtaining $s_0(x)$;
(iii) compute $q(x), x \in (0, b)$ from (17).

The computation of the integrals in (19) and (20) on step (i) as well as the differentiation of $s_0(x)$ on step (ii) were performed similarly to [3].

Example 2 Consider a test problem with

$$q(x) = \frac{1200e^{10x}}{(6e^{10x} - 1)^2}, \quad x > 0.$$  

The Jost solution is given by [14]

$$e(\rho, x) = e^{ix} \left( \frac{10i}{\rho + 5i} - \frac{1}{6e^{10x} - 1} \right), \quad x > 0.$$  

Hence $F(\rho) = (\rho + 7i) / (\rho + 5i)$, and the discrete spectrum is empty.

With 1201 points $\{x_l\}$ uniformly distributed on the interval $[0, \pi]$ the maximal error of approximation of the potential $q$ by the recovered potential denoted by $q_M$ is reported in Table 1. Here $M$ corresponds to the number of the equations in a truncated system obtained from (18):

$$\frac{s_m(x)}{4m + 3} + \sum_{n=0}^{M} s_n(x)B_{m,n}(x) = -f_m(x, x), \quad \text{for all } m = 0, \ldots, M. \quad (25)$$

| $M$  | $\max_{x \in (0, \pi)} |q(x) - q_M(x)|$ |
|------|-----------------------------------|
| 0    | 0.165                             |
| 1    | 0.016                             |
| 2    | 0.0037                            |
| 3    | 0.0012                            |
| 4    | $2.19 \times 10^{-4}$            |
| 5    | $1.31 \times 10^{-5}$            |
| 6    | $6.5 \times 10^{-6}$             |
| 7    | $5.8 \times 10^{-6}$             |

Thus, even a reduced number of equations in (25) is sufficient for recovering the potential with a satisfactory accuracy.
6. Conclusions

The classical inverse quantum scattering problem is considered. From the corresponding Gel’fand-Levitan equation a system of linear algebraic equations is derived for the coefficients of the Fourier-Legendre series expansion of the output (transmutation operator) kernel. It is shown that the knowledge of the very first coefficient is sufficient for recovering the potential and hence for solving the inverse problem. A numerical illustration is presented. The proposed method for solving the inverse quantum scattering problem turns to be quite universal. In [1], [3] and [2] it was developed for solving the inverse Sturm-Liouville problem on a finite interval, on a half line and the inverse scattering problem on the line, respectively. Two key ingredients are necessary for its application: the availability of an appropriate Povzner-Levitan-Marchenko type transmutation operator and a corresponding Gel’fand-Levitan type integral equation.

It is worth emphasizing that the Gel’fand-Levitan equation itself is not aimed to be solved. It is used for writing down a system of linear algebraic equations for the coefficients of a series expansion of the transmutation kernel, and, since the potential is recovered from the very first coefficient, a reduced number of equations in the truncated system is enough for obtaining excellent numerical results. The method is direct and simple, and can be considered for a homework exercise to an undergraduate student.

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References

[1] Kravchenko V V 2019 *J. Inverse Ill-Posed Probl* **27** 401
[2] Kravchenko V V 2019 *Math. Meth. Appl. Sci.* **42** 1321
[3] Delgado B B, Khmelnytskaya K V and Kravchenko V V 2019 *Math. Meth. Appl. Sci.* **42** 7359
[4] Kravchenko V V, Navarro L J and Torba S M 2017 *Appl. Math. Comput.* **314** 173
[5] Freiling G, Mazur T and Yurko V A 2007 *Adv. Dynam. Syst. Appl.* **2** 95
[6] Chadan Kh and Sabatier P C 1989 *Inverse problems in quantum scattering theory* (Berlin: Springer)
[7] Freiling G and Yurko V A 2001 *Inverse Sturm-Liouville problems and their applications* (New York: Nova Science Publishers, Inc.)
[8] Yurko V A 2007 *Introduction to the theory of inverse spectral problems* (Moscow: Fizmatlit) (in Russian)
[9] Delgado B B, Khmelnytskaya K V and Kravchenko V V 2019 *Math. Meth. Appl. Sci.* https://doi.org/10.1002/mma.5881
[10] Levitan B M 1987 *Inverse Sturm-Liouville problems* (Zeist: VSP)
[11] Kirst Th, von Geramb H V and Amos K A 1990 *Z. Phys. A* **336** 365
[12] Prudnikov A P, Brychkov Yu A and Marichev O I 1986 *Integrals and series. Vol. 2. Special functions* (New York: Gordon & Breach Science Publishers)
[13] Akhiezer N I and Glazman I M 1993 *Theory of Linear Operators in Hilbert Space* (New York: Dover)
[14] Aktosun T 2004 *Inverse Probl.* **20** 859