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Krein's method in inverse scattering *†‡

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Abstract

A detailed discussion of the Krein's results (applicable for solving the inverse scattering problem) is given with complete proofs.

It is shown that the S-function $S(k)$ used in Krein's work is the S-matrix used in physics.

The basic new results of the paper include the detailed description and analysis of an inversion algorithm based on Krein's results and a proof of its consistency, that is the proof that the reconstructed potential generates the same scattering data from which it was reconstructed.

Numerical advantages of using Krein's method are discussed.

1 Introduction

The inverse scattering problem on half-axis consists of finding

$$q(x) \in L_{1,1} = \left\{ q : q = \overline{q}, \quad \int_0^\infty x|q(x)|dx < \infty \right\}$$

from the knowledge of the scattering data

$$\mathcal{S} := \{S(k), k_j, s_j, 1 \leq j \leq J\}. \tag{1.1}$$

Here

$$S(k) := \frac{f(-k)}{f(k)}$$

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is the S-matrix, $f(k)$ is the Jost function

$$f(k) := f(0,k), \tag{1.2}$$

$f(x,k)$ is the solution to the equation

$$\ell f := f'' + k^2 f - q(x)f = 0 \tag{1.3}$$

which is uniquely defined by the condition

$$f(x,k) = e^{ikx} + o(1), \quad x \to +\infty, \tag{1.4}$$

$k_j > 0$ are the (only) zeros of $f(x)$ in the region $\mathbb{C}_+ := \{k : \operatorname{Im} k > 0\}$, $-k_j^2$ are the negative eigenvalues of the Dirichlet operator $-\frac{d^2}{dx^2} + q(x)$ on $(0,\infty)$, $s_j > 0$ are the norming constants:

$$s_j = -\frac{2ik_j}{\dot{f}(ik_j) f'(0,ik_j)}, \tag{1.5}$$

and $J \geq 0$ is the number of the negative eigenvalues.

For simplicity *we assume that there are no bound states.* This assumption is removed in section 4.

This paper is a commentary to Krein's paper [?]. It contains not only a detailed proof of the results announced in [?] but also a proof of the new results not mentioned in [?]. In particular, it contains an analysis of the invertibility of the steps in the inversion procedure based on Krein's results, and a proof of the consistency of this procedure, that is, a proof of the fact that the reconstructed potential generates the scattering data from which it was reconstructed. A numerical scheme for solving inverse scattering problem, based on Krein's inversion method, is proposed, and its advantages compared with the Marchenko and Gel'fand-Levitan methods are discussed. Some of the results are stated in Theorems 1.1 – 1.4 below.

Consider the equation

$$(I + H_x)\Gamma_x := \Gamma_x(t,s) + \int_0^x H(t-u)\Gamma_x(u,s)du = H(t-s), \quad 0 \leq t,s \leq x. \tag{1.6}$$

Equation (1.6) shows that $\Gamma_x = (I+H_x)^{-1}H = I - (I+H_x)^{-1}$, so

$$(I + H_x)^{-1} = I - \Gamma_x \tag{1.6$'$}$$

in operator form, and

$$H_x = (I - \Gamma_x)^{-1} - I. \tag{1.6$''$}$$

Let us assume that $H(t)$ is a real-valued even function

$$H(-t) = H(t), \quad H(t) \in L^1(\mathbb{R}) \cap L^2(\mathbb{R}),$$

$$1 + \widetilde{H}(k) > 0, \quad \widetilde{H}(k) := \int_{-\infty}^{\infty} H(t)e^{ikt}dt = 2\int_0^{\infty} \cos(kt)H(t)dt. \tag{1.7}$$

Then (1.6) is uniquely solvable for any $x > 0$, and there exists a limit

$$\Gamma(t,s) = \lim_{x\to\infty} \Gamma_x(t,s) := \Gamma_\infty(t,s), \quad t,s \geq 0, \tag{1.8}$$

where $\Gamma(t,s)$ solves the equation

$$\Gamma(t,s) + \int_0^{\infty} H(t-u)\Gamma(u,s)du = H(t-s), \quad 0 \leq t,s < \infty. \tag{1.9}$$

Given $H(t)$, one solves (1.6), finds $\Gamma_{2x}(s,0)$, then defines

$$\psi(x,k) := \frac{E(x,k) - E(x,-k)}{2i}, \tag{1.10}$$

where

$$E(x,k) := e^{ikx}\left[1 - \int_0^{2x} \Gamma_{2x}(s,0)e^{-iks}ds\right]. \tag{1.11}$$

Formula (1.11) gives a one-to-one correspondence between $E(x,k)$ and $\Gamma_{2x}(s,0)$.

Remark 1.1. *In [1] $\Gamma_{2x}(0,s)$ is used in place of $\Gamma_{2x}(s,0)$ in the definition of $E(x,k)$. By formula (2.21) (see section 2 below) one has $\Gamma_x(0,x) = \Gamma_x(x,0)$, but $\Gamma_x(0,s) \neq \Gamma_x(s,0)$ in general. The theory presented below cannot be constructed with $\Gamma_{2x}(0,s)$ in place of $\Gamma_{2x}(s,0)$ in formula (1.11).*

Note that

$$E(x,k) = e^{ikx}f(-k) + o(1), \quad x \to +\infty, \tag{1.12}$$

where

$$f(k) := 1 - \int_0^{\infty} \Gamma(s)e^{iks}ds, \tag{1.13}$$

and

$$\Gamma(s) := \lim_{x\to+\infty} \Gamma_x(s,0) := \Gamma_\infty(s,0). \tag{1.14}$$

Furthermore,

$$\psi(x,k) = \frac{e^{ikx}f(-k) - e^{-ikx}f(k)}{2i} + o(1), \quad x \to +\infty, \tag{1.15}$$

and

$$\psi(x,k) = |f(k)|\sin(kx + \delta(k)) + o(1), \quad x \to +\infty,$$

where

$$f(k) = |f(k)|e^{-i\delta(k)}, \quad \delta(k) = -\delta(-k), \quad k \in \mathbb{R}.$$

The function $\delta(k)$ is called the phase shift. One has $S(k) = e^{2i\delta(k)}$.

We have changed the notations from [?] in order to show the physical meaning of the quantity (1.12): $f(k)$ is the Jost function of the scattering theory. The function $\frac{\psi(x,k)}{f(k)}$ is the solution to the scattering problem: it solves equation (1.3), and satisfies the correct boundary conditions: $\frac{\psi(0,k)}{f(k)} = 0$, and $\frac{\psi(x,k)}{f(k)} = e^{i\delta(k)} \sin(kx + \delta(k)) + o(1)$ as $x \to \infty$.

Krein [?] calls

$$S(k) := \frac{f(-k)}{f(k)} \tag{1.16}$$

the S-function, and we will show that (1.16) is the S-matrix used in physics.

yyAssuming no bound states, one can solve *the inverse scattering problem (ISP):*

given $S(k)$ $\forall k > 0$, find $q(x)$.

A solution of the ISP, based on the results of [?], consists of four steps:

1) Given $S(k)$, find $f(k)$ by solving the Riemann problem (2.37).

2) Given $f(k)$, calculate $H(t)$ using the formula

$$1 + \widetilde{H} = 1 + \int_{-\infty}^{\infty} H(t) e^{ikt} dt = \frac{1}{|f(k)|^2}. \tag{1.17}$$

3) Given $H(t)$, solve (1.6) and find $\Gamma_x(t,s)$ and then $\Gamma_{2x}(2x,0)$, $0 \le x < \infty$.

4) Define

$$a(x) = 2\Gamma_{2x}(2x,0), \tag{1.18}$$

where

$$a(0) = 2H(0), \tag{1.18$'$}$$

and calculate the potential

$$q(x) = a^2(x) + a'(x), \quad a(0) = 2H(0). \tag{1.19}$$

One can also calculate $q(x)$ by the formula:

$$q(x) = 2\frac{d}{dx}[\Gamma_{2x}(2x,0) - \Gamma_{2x}(0,0)]. \tag{1.19$'$}$$

Indeed, $2\Gamma_{2x}(2x,0) = a(x)$, see (1.18), $\frac{d}{dx}\Gamma_{2x}(0,0) = -2\Gamma_{2x}(2x,0)\Gamma_{2x}(0,2x)$, see (2.22), and $\Gamma_{2x}(2x,0) = \Gamma_{2x}(0,2x)$, see (2.21).

There is an alternative (known) way, based on the Wiener-Levy theorem, to do step 1):

Given $S(k)$, find $\delta(k)$, the phase shift, then calculate the function

$$g(t) := -\frac{2}{\pi}\int_0^{\infty} \delta(k)\sin(kt)dk,$$

and finally calculate

$$f(k) = \exp\left(\int_0^\infty g(t)e^{ikt}dk\right).$$

The potential $q \in L_{1,1}$ generates the S-matrix $S(k)$ with which we started provided that the following conditions (1.20) -(1.22) hold:

$$S(k) = \overline{S(-k)} = S^{-1}(k), \quad k \in \mathbb{R}, \tag{1.20}$$

the overbar stands for complex conjugation,

and

$$ind_{\mathbb{R}} S(k) = 0, \tag{1.21}$$

$$||F(x)||_{L^\infty(\mathbb{R}_+)} + ||F(x)||_{L^1(\mathbb{R}_+)} + ||xF'(x)||_{L^1(\mathbb{R}_+)} < \infty, \tag{1.22}$$

where

$$F(x) := \frac{1}{2\pi}\int_{-\infty}^\infty [1 - S(k)]e^{ikx}dk. \tag{1.23}$$

By the index (1.21) one means the increment of the argument of $S(k)$ (when k runs from $-\infty$ to $+\infty$ along the real axis) divided by 2π. The function (1.10) satisfies the equation

$$\psi'' + k^2\psi - q(x)\psi = 0, \quad x \in \mathbb{R}_+. \tag{1.24}$$

Recall that *we have assumed that there are no bound states.*

In section 2 the above method is justified and the following theorems are proved:

Theorem 1.1. *If (1.20)-(1.22) hold, then $q(x)$ defined by (1.19) is the unique solution to ISP and this $q(x)$ has $S(k)$ as the scattering matrix.*

Theorem 1.2. *The function $f(k)$, defined by (1.13), is the Jost function corresponding to potential (1.19).*

Theorem 1.3. *Condition (1.7) implies that equation (1.6) is solvable for all $x \geq 0$ and its solution is unique.*

Theorem 1.4. *If condition (1.7) holds, then relation (1.14) holds and $\Gamma(s) := \Gamma_\infty(s, 0)$ is the unique solution to the equation*

$$\Gamma(s) + \int_0^\infty H(s-u)\Gamma(u)du = H(s), \quad s \geq 0. \tag{1.25}$$

The diagram explaining the inversion method for solving ISP, based on Krein's results from [?], can be shown now:

$$S(k) \underset{s_1}{\overset{(2.38)}{\Rightarrow}} f(k) \underset{s_2}{\overset{(1.17)}{\Rightarrow}} H(t) \underset{s_3}{\overset{(1.6)}{\Rightarrow}} \Gamma_x(t,s) \underset{s_4}{\overset{\text{(trivial)}}{\Rightarrow}} \Gamma_{2x}(2x, 0) \underset{s_5}{\overset{(1.18)}{\Rightarrow}} a(x) \underset{s_6}{\overset{(1.19)}{\Rightarrow}} q(x). \tag{1.26}$$

In this diagram s_m denotes step number m. Steps s_2, s_4, s_5 and s_6 are trivial. Step s_1 is almost trivial: it requires solving a Riemann problem with index zero and can be done analytically, in closed form. Step s_3 is the basic (non-trivial) step which requires solving a family of Fredholm-type linear integral equations (1.6). These equations are uniquely solvable if assumption (1.7) holds, or if assumptions (1.20)-(1.22) hold.

We analyze in section 2 the invertibility of the steps in diagram (1.26). Note also that, if one assumes (1.20)-(1.22), diagram (1.26) can be used for solving the inverse problems of finding $q(x)$ from the following data:

a) from $f(k)$, $\forall k > 0$,

b) from $|f(k)|^2$, $\forall k > 0$, or

c) from the spectral function $d\rho(\lambda)$.

Indeed, if (1.20)-(1.22) hold, then a) and b) are contained in diagram (1.26), and c) follows from the known formula (e.g., [**?**], p.256)

$$d\rho(\lambda) = \begin{cases} \frac{\sqrt{\lambda}}{\pi} \frac{d\lambda}{|f(\sqrt{\lambda})|^2}, & \lambda > 0, \\ 0, & \lambda < 0. \end{cases} \tag{1.27}$$

Let $\lambda = k^2$. Then (still assuming (1.21)) one has:

$$d\rho = \frac{2k^2}{\pi} \frac{1}{|f(k)|^2} dk, \quad k > 0. \tag{1.28}$$

Note that the general case of the inverse scattering problem on the half-axis, when

$$\text{ind}_{\mathbb{R}} S(k) := \nu \neq 0,$$

can be reduced to the case $\nu = 0$ by the procedure described in section 4 provided that $S(k)$ is the $S-$matrix corresponding to a potential $q \in L_{1,1}(\mathbb{R}_+)$. Necessary and sufficient conditions for such an $S(k)$ are conditions (1.20)-(1.22) (see [4]).

Section 3 contains a discussion of the numerical aspects of the inversion procedure based on Krein's method. There are advantages in using this procedure (as compared with the Gel'fand-Levitan procedure): integral equation (1.6), solving of which constitutes the basic step in the Krein inversion method, is a Fredholm convolution-type equation. Solving such an equation numerically leads to inversion of Toeplitz matrices, which can be done efficiently and with much less computer time than solving the Gel'fand-Levitan equation (5.3). Combining Krein's and Marchenko's inversion methods yields the most efficient way to solve inverse scattering problems.

Indeed, for small x equation (1.6) can be solved by iterations since the norm of the integral operator in (1.6) is less than 1 for sufficiently small x, say $0 < x < x_0$. Thus $q(x)$ can be calculated for $0 \leq x \leq \frac{x_0}{2}$ by diagram (1.26).

For $x > 0$ one can solve by iterations Marchenko's equation for the kernel $A(x, y)$:

$$A(x, y) + F(x + y) + \int_x^\infty A(x, s)F(s + y)ds = 0, \quad 0 \le x \le y < \infty, \tag{1.29}$$

where, if (1.21) holds, the known function $F(x)$ is defined by the formula:

$$F(x) := \frac{1}{2\pi} \int_{-\infty}^{\infty} [1 - S(k)]e^{ikx}dk. \tag{1.30}$$

Indeed, for $x > 0$ the norm of the operator in (1.29) is less than 1 ([?]) and it tends to 0 as $x \to +\infty$.

Finally let us discuss the following question: in the justification of both the Gel'fand-Levitan and Marchenko methods, the eigenfunction expansion theorem and the Parseval relation play the fundamental role. In contrast, the Krein method apparently does not use the eigenfunction expansion theorem and the Parseval relation. However, implicitly, this method is also based on such relations. Namely, assumption (1.7) implies that the function $S(k)$, that is, the S-matrix corresponding to the potential (1.19), has index 0. If, in addition, this potential is in $L_{1,1}(\mathbb{R}_+)$, then conditions (1.20) and (1.22) are satisfied as well, and the eigenfunction expansion theorem and Parseval's equality hold. Necessary and sufficient conditions, imposed directly on the function $H(t)$, which guarantee that conditions (1.20)-(1.22) hold, are not known. However, from the results of section 2 it follows that conditions (1.20)-(1.22) hold if and only if $H(t)$ is such that the diagram (1.26) leads to a $q(x) \in L_{1,1}(\mathbb{R}_+)$. Alternatively, conditions (1.20)-(1.22) hold (and consequently, $q(x) \in L_{1,1}(\mathbb{R}_+)$) if and only if condition (1.7) holds and the function $f(k)$, which is uniquely defined as the solution to the Riemann problem

$$\Phi_+(k) = [1 + \widetilde{H}(k)]^{-1}\Phi_-(k), \quad k \in \mathbb{R}, \tag{1.31}$$

by the formula

$$f(k) = \Phi_+(k), \tag{1.32}$$

generates the S-matrix $S(k)$ (by formula (1.16)), and this $S(k)$ satisfies conditions (1.20)-(1.22). Although the above conditions are verifiable in principle, they are not satisfactory because they are implicit, they are not formulated in terms of structural properties of the function $H(t)$ (such as smoothness, rate of decay, etc.).

In section 2 Theorems 1.1 – 1.4 are proved. In section 3 numerical aspects of the inversion method based on Krein's results are discussed. In section 4 the ISP with bound states is discussed. In section 5 a relation between Krein's and Gel'fand-Levitan's methods is explained.

2 Proofs

Proof of Theorem 1.3. If $v \in L^2(0, x)$, then

$$(v + H_x v, v) = \frac{1}{2\pi}[(\widetilde{v}, \widetilde{v})_{L^2(\mathbb{R})} + (\widetilde{H}\widetilde{v}, \widetilde{v})_{L^2(\mathbb{R})}] \tag{2.1}$$

where the Parseval equality was used,

$$\widetilde{v} := \int_0^x v(s)e^{iks}ds,$$

$$(v,v) = \int_0^x |v|^2 ds = (v,v)_{L^2(\mathbb{R})}. \tag{2.2}$$

Thus $I + H_x$ is a positive definite selfadjoint operator in the Hilbert space $L^2(0,x)$ if (1.7) holds. Note that, since $H(t) \in L^1(\mathbb{R})$, one has $\widetilde{H}(k) \to 0$ as $|k| \to \infty$, so (1.7) implies

$$1 + \widetilde{H}(k) \geq c > 0. \tag{2.3}$$

A positive definite selfadjoint operator in a Hilbert space is boundedly invertible. Theorem 1.3 is proved. □

Note that our argument shows that

$$||(I + H_x)^{-1}||_{L^2(\mathbb{R})} \leq c^{-1}. \tag{2.4}$$

Before we prove Theorem 1.4, let us prove a simple lemma. For results of this type, see [?].

Lemma 2.1. *If (1.7) holds, then the operator*

$$H\varphi := \int_0^\infty H(t-u)\varphi(u)du \tag{2.5}$$

is a bounded operator in $L^p(\mathbb{R}_+)$*,* $p = 1, 2, \infty$*.*

For $\Gamma_x(u,s) \in L^1(\mathbb{R}_+)$ *one has*

$$|| \int_x^\infty du H(t-u)\Gamma_x(u,s)||_{L^2(0,x)} \leq c_1 \int_x^\infty du|\Gamma_x(u,s)|. \tag{2.6}$$

Proof. Let $||\varphi||_p := ||\varphi||_{L^p(\mathbb{R}_+)}$. One has

$$||H\varphi||_1 \leq \sup_{u\in\mathbb{R}_+} \int_0^\infty dt|H(t-u)| \int_0^\infty |\varphi(u)|du \leq \int_{-\infty}^\infty |H(s)|ds||\varphi||_1 = 2||H||_1\, ||\varphi||_1, \tag{2.7}$$

where we have used the assumption $H(t) = H(-t)$. Similarly,

$$||H\varphi||_\infty \leq 2||H||_1\, ||\varphi||_\infty. \tag{2.8}$$

Finally, using Parseval's equality, one gets:

$$2\pi||H\varphi||_2^2 = ||\widetilde{H}\tilde{\varphi}_+||^2_{L^2(\mathbb{R})} \leq \sup_{k\in\mathbb{R}} |\widetilde{H}(k)|^2||\varphi||_2^2, \tag{2.9}$$

where

$$\varphi_+(x) := \begin{cases} \varphi(x), & x \geq 0, \\ 0, & x < 0. \end{cases} \tag{2.10}$$

Since $|\widetilde{H}(k)| \leq 2||H||_1$ one gets from (2.9) the estimate:

$$||H\varphi||_2 \leq \sqrt{2/\pi}||H||_1 \; ||\varphi||_2. \tag{2.11}$$

To prove (2.6), one notes that

$$\int_0^x dt|\int_x^\infty duH(t-u)\Gamma_x(u,s)|^2 \leq \sup_{u,v\geq x}\int_0^x dt|H(t-u)H(t-v)|(\int_x^\infty |\Gamma_x(u,s)|du)^2$$

$$\leq c_1(\int_x^\infty du|\Gamma_x(u,s)|)^2.$$

Estimate (2.6) is obtained. Lemma 2.1 is proved. □

Proof of Theorem 1.4. Define $\Gamma_x(t,s) = 0$ for t or s greater than x. Let $w := \Gamma_x(t,s) - \Gamma(t,s)$. Then (1.6) and (1.9) imply

$$(I + H_x)w = \int_x^\infty H(t-u)\Gamma(u,s)du := h_x(t,s). \tag{2.12}$$

If condition (1.7) holds, then equations (1.9) and (1.25) have solutions in $L^1(\mathbb{R}_+)$, and, since $\sup_{t\in\mathbb{R}}|H(t)| < \infty$, it is clear that this solution belongs to $L^\infty(\mathbb{R}_+)$, and, consequently, to $L^2(\mathbb{R}_+)$, because $||\varphi||_2 \leq ||\varphi||_\infty||\varphi||_1$. The proof of Theorem 1.3 shows that such a solution is unique and does exist. From (2.4) one gets

$$\sup_{x\geq 0}||(I+H_x)^{-1}||_{L^2(0,x)} \leq c^{-1}. \tag{2.13}$$

For any fixed $s > 0$, in particular, for $s = 0$ in Theorem 1.4, one sees that $\sup_{x\geq y}||h_x(t,s)|| \to 0$ as $y \to \infty$, where the norm here stands for any of the three norms $L^p(0,x), p = 1,2,\infty$. Therefore (2.12) and (2.11) imply

$$\begin{aligned} ||w||^2_{L^2(0,x)} &\leq c^{-2}||h_x||^2_{L^2(0,x)} \\ &\leq c^{-2}\left\|\int_x^\infty H(t-u)\Gamma(u,s)du\right\|_{L^1(0,x)}\left\|\int_x^\infty H(t-u)\Gamma(u,s)du\right\|_{L^\infty(0,x)} \\ &\leq \text{ const } \|\Gamma(u,s)\|^2_{L^1(x,\infty)} \to 0 \text{ as } x\to\infty, \end{aligned} \tag{2.14}$$

since $\Gamma(u,s) \in L^1(\mathbb{R}_+)$ for any fixed $s > 0$ and $H(t) \in L^1(\mathbb{R})$.

Also

$$\begin{aligned} \|w(t,s)\|^2_{L^\infty(0,x)} \leq 2(||h_x||^2_{L^\infty(0,x)} + ||H_xw||^2_{L^\infty(0,x)}) \leq \\ c_1||\Gamma(u,s)||^2_{L^1(x,\infty)} + c_2\sup_{t\in\mathbb{R}}||H(t-u)||^2_{L^2(0,x)}||w||^2_{L^2(0,x)}, \end{aligned} \tag{2.15}$$

where $c_j > 0$ are some constants. Finally, by (2.6), one has:

$$\|w(t,s)\|^2_{L^2(0,x)} \leq c_3(\int_x^\infty |\Gamma(u,s)|du)^2 \to 0 \text{ as } x \to +\infty. \tag{2.16}$$

From (2.15) and (2.16) relation (1.14) follows. Theorem 1.4 is proved. □

Let us now prove Theorem 1.2. We need several lemmas.

Lemma 2.2. *The function (1.11) satisfies the equations*

$$E' = ikE - a(x)E_-, \quad E(0,k) = 1, \quad E_- := E(x,-k), \tag{2.17}$$

$$E'_- = -ikE_- - a(x)E, \quad E_-(0,k) = 1, \tag{2.18}$$

where $E' = \frac{dE}{dx}$*, and* $a(x)$ *is defined in (1.18).*

Proof. Differentiate (1.11) and get

$$E' = ikE - e^{ikx}\left(2\Gamma_{2x}(2x,0)e^{-ik2x} + 2\int_0^{2x} \frac{\partial \Gamma_{2x}(s,0)}{\partial(2x)} e^{-iks}ds\right). \tag{2.19}$$

We will check below that

$$\frac{\partial\ \Gamma_x(t,s)}{\partial x} = -\Gamma_x(t,x)\Gamma_x(x,s), \tag{2.20}$$

and

$$\Gamma_x(t,s) = \Gamma_x(x-t, x-s). \tag{2.21}$$

Thus, by (2.20),

$$\frac{\partial \Gamma_{2x}(s,0)}{\partial(2x)} = -\Gamma_{2x}(s,2x)\Gamma_{2x}(2x,0). \tag{2.22}$$

Therefore (2.19) can be written as

$$E' = ikE - e^{-ikx}a(x) + a(x)e^{ikx}\int_0^{2x}\Gamma_{2x}(s,2x)e^{-iks}ds. \tag{2.23}$$

By (2.21) one gets

$$\Gamma_{2x}(s,2x) = \Gamma_{2x}(2x-s,0). \tag{2.24}$$

Thus

$$\begin{aligned} e^{ikx}\int_0^{2x}\Gamma_{2x}(s,2x)e^{-iks}ds &= \int_0^{2x}\Gamma_{2x}(2x-s,0)e^{ik(x-s)}ds \\ &= e^{-ikx}\int_0^{2x}\Gamma_{2x}(y,0)e^{iky}dy. \end{aligned} \tag{2.25}$$

From (2.23) and (2.25) one gets (2.17).

Equation (2.18) can be obtained from (2.17) by changing k to $-k$. Lemma 2.2 is proved if formulas (2.20)-(2.21) are checked.

To check (2.21), use $H(-t) = H(t)$ and compare the equation for $\Gamma_x(x-t, x-s) := \varphi$,

$$\Gamma_x(x-t, x-s) + \int_0^x H(x-t-u)\Gamma_x(u, x-s)du = H(x-t-x+s) = H(t-s), \quad (2.26)$$

with equation (1.6). Let $u = x - y$. Then (2.26) can be written as

$$\varphi + \int_0^x H(t-y)\varphi\, dy = H(t-s), \quad (2.27)$$

which is equation (1.6) for φ. Since (1.6) has at most one solution, as we have proved above (Theorem 1.3), formula (2.21) is proved.

To prove (2.20), differentiate (1.6) with respect to x and get:

$$\Gamma'_x(t, s) + \int_0^x H(t-u)\Gamma'_x(u, s)du = -H(t-x)\Gamma_x(x, s), \quad \Gamma'_x := \frac{\partial \Gamma_x}{\partial x}. \quad (2.28)$$

Set $s = x$ in (1.6), multiply (1.6) by $-\Gamma_x(x, s)$, compare with (2.28) and use again the uniqueness of the solution to (1.6). This yields (2.20).

Lemma 2.2 is proved. □

Lemma 2.3. *Equation (1.24) holds.*

Proof. From (1.10) and (2.17)-(2.18) one gets

$$\psi'' = \frac{E'' - E''_-}{2i} = \frac{(ikE - a(x)E_-)' - (-ikE_- - a(x)E)'}{2i}. \quad (2.29)$$

Using (2.17)-(2.18) again one gets

$$\psi'' = -k^2\psi + q(x)\psi, \quad q(x) := a^2(x) + a'(x). \quad (2.30)$$

Lemma 2.3 is proved. □

Proof of Theorem 1.2. The function ψ defined in (1.10) solves equation (1.24) and satisfies the conditions

$$\psi(0, k) = 0, \quad \psi'(0, k) = k. \quad (2.31)$$

The first condition is obvious (in [**?**] there is a *misprint:* it is written that $\psi(0, k) = 1$), and the second condition follows from (1.10) and (2.15):

$$\psi'(0, k) = \frac{E'(0, k) - E'_-(0, k)}{2i} = \frac{ikE - aE_- - (ikE_- - aE)}{2i}\Bigg|_{x=0} = \frac{2ik}{2i} = k.$$

Let $f(x,k)$ be the Jost solution to (1.24) which is uniquely defined by the asymptotics

$$f(x,k)=e^{ikx}+o(1), \quad x\to+\infty. \tag{2.32}$$

Since $f(x,k)$ and $f(x,-k)$ are linearly independent, one has

$$\psi=c_1 f(x,k)+c_2 f(x,-k), \tag{2.33}$$

where c_1, c_2 are some constants independent of x but depending on k.

From (2.31) and (2.33) one gets

$$c_1=\frac{f(-k)}{2i}, \quad c_2=\frac{-f(k)}{2i}; \quad f(k):=f(0,k). \tag{2.34}$$

Indeed, the choice of c_1 and c_2 guarantees that the first condition (2.31) is obviously satisfied, while the second follows from the Wronskian formula:

$$f'(0,k)f(-k)-f(k)f'(0,-k)=2ik. \tag{2.35}$$

From (2.32), (2.33) and (2.34) one gets:

$$\psi(x,k)=e^{ikx}f(-k)-e^{-ikx}f(k)+o(1), \quad x\to+\infty. \tag{2.36}$$

Comparing (2.36) with (1.15) yields the conclusion of Theorem 1.2. □

Invertibility of the steps of the inversion procedure. Proof of Theorem 1.1

Let us start with a discussion of the inversion steps 1) – 4) described in the introduction.

Then we discuss the uniqueness of the solution to ISP and the consistency of the inversion method, that is, the fact that $q(x)$, reconstructed from $S(k)$ by steps 1) – 4), generates the original $S(k)$.

Let us go through steps 1) – 4) of the reconstruction method and prove their invertibility. The consistency of the inversion method follows from the invertibility of the steps of the inversion method.

Step 1. $S(k)\Rightarrow f(k)$.

Assume $S(k)$ satisfying (1.20)-(1.22) is given. Then solve the Riemann problem

$$f(k)=S(-k)f(-k), \qquad k\in\mathbb{R}. \tag{2.37}$$

Since $\mathrm{ind}_{\mathbb{R}}S(k)=0$, one has $\mathrm{ind}_{\mathbb{R}}S(-k)=0$. Therefore the problem (2.37) of finding an analytic function $f_+(k)$ in $\mathbb{C}_+:=\{k:\ \mathrm{Im}\,k>0\}$, $f(k):=f_+(k)$ in $\mathbb{C}_+$, and and analytic function $f_-(k):=f(-k)$ in $\mathbb{C}_-:=\{k:\ \mathrm{Im}\,k<0\}$ from equation (2.37) can be solved in closed form. Namely, define

$$f(k)=\exp\left\{\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{\ln S(-y)dy}{y-k}\right\}, \quad \mathrm{Im}\,k>0. \tag{2.38}$$

Then $f(k)$ solves (2.37), $f_+(k) = f(k)$, $f_-(k) = f(-k)$. Indeed,

$$\ln f_+(k) - \ln f_-(k) = \ln S(-k), \quad k \in \mathbb{R} \tag{2.39}$$

by the known jump formula for the Cauchy integral. Integral (2.38) converges absolutely at infinity, $\ln S(-y)$ is differentiable with respect to y for $y \neq 0$, and is bounded on the real axis, so the Cauchy integral in (2.38) is well defined.

To justify the above claims, one uses the known properties of the Jost function

$$f(k) = 1 + \int_0^\infty A(0,y)e^{iky}dy := 1 + \int_0^\infty A(y)e^{iky}dy, \tag{2.40}$$

where (see [**?**])

$$|A(y)| \leq c \int_{\frac{y}{2}}^\infty |q(t)|dt, \tag{2.41}$$

$$\left| \frac{\partial A(y)}{\partial y} + \frac{1}{4} q\left(\frac{y}{2}\right) \right| \leq c \int_{\frac{y}{2}}^\infty |q(t)|dt, \tag{2.42}$$

$c > 0$ stand for various constants and $A(y)$ is a real-valued function. Thus

$$f(k) = 1 - \frac{A(0)}{ik} - \frac{1}{ik} \int_0^\infty A'(t)e^{ikt}dt, \tag{2.43}$$

$$S(-k) = \frac{f(k)}{f(-k)} = \frac{1 - \frac{A(0)}{ik} - \frac{1}{ik}\widetilde{A}'(k)}{1 + \frac{A(0)}{ik} + \frac{1}{ik}\widetilde{A}'(-k)} = 1 + 0\left(\frac{1}{k}\right). \tag{2.44}$$

Therefore

$$\ln S(-k) = 0\left(\frac{1}{k}\right) \quad \text{as} \quad |k| \to \infty, \quad k \in \mathbb{R}. \tag{2.45}$$

Also

$$\dot{f}(k) = i \int_0^\infty A(y)ye^{iky}dy, \quad \dot{f} := \frac{\partial f}{\partial k}. \tag{2.46}$$

Estimate (2.41) implies

$$\int_0^\infty y|A(y)|dy \leq 2 \int_0^\infty t|q(t)|dt < \infty, \quad A(y) \in L^2(\mathbb{R}_+), \tag{2.47}$$

so that $\dot{f}(k)$ is bounded for all $k \in \mathbb{R}$, $f(k) - 1 \in L^2(\mathbb{R})$, $S(-k)$ is differentiable for $k \neq 0$, and $\ln S(-y)$ is bounded on the real axis, as claimed. Note that

$$f(-k) = \overline{f(k)}, \quad k \in \mathbb{R}. \tag{2.48}$$

The converse step

$$f(k) \Rightarrow S(k)$$

is trivial:

$$S(k) = \frac{f(-k)}{f(k)}.$$

If $\mathrm{ind}_{\mathbb{R}} S = 0$ then $f(k)$ is analytic in $\mathbb{C}_+$, $f(k) \neq 0$ in $\mathbb{C}_+$, $f(k) = 1 + O\left(\frac{1}{k}\right)$ as $|k| \to \infty$, $k \in \mathbb{C}_+$, and (2.48) holds.

Step 2. $f(k) \Rightarrow H(t)$.

This step is done by formula (1.17):

$$H(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikt} \left(\frac{1}{|f(k)|^2} - 1 \right) dk. \tag{2.49}$$

One has $H \in L^2(\mathbb{R})$. Indeed, it follows from (2.43) that

$$|f(k)|^2 - 1 = -\frac{2}{k} \int_0^{\infty} A'(t) \sin(kt) dt + O\left(\frac{1}{|k|^2} \right), \quad |k| \to \infty, \quad k \in \mathbb{R}. \tag{2.50}$$

The function

$$w(k) := \frac{1}{k} \int_0^{\infty} A'(t) \sin(kt) dt \tag{2.51}$$

is continuous because $A'(t) \in L^1(\mathbb{R}_+)$ by (2.42), and $w \in L^2(\mathbb{R})$ since $w = o\left(\frac{1}{|k|}\right)$ as $|k| \to \infty$, $k \in \mathbb{R}$. Thus, $H \in L^2(\mathbb{R})$.

Also, $H \in L^1(\mathbb{R})$. Indeed, integrating by parts, one gets from (2.49) the relation: $2\pi H(t) = \frac{i}{t} \int_{-\infty}^{\infty} e^{-ikt} [\dot{f}(k) f(-k) - \dot{f}(-k) f(k)] \frac{dk}{|f(k)|^4} := \frac{i}{t} g(t)$, and $g \in L^2(\mathbb{R})$, therefore $H \in L^1(\mathbb{R})$. To check that $g \in L^2(\mathbb{R})$, one uses (2.40)-(2.42) and (2.46)-(2.47), to conclude that $[\dot{f}(k) f(-k) - \dot{f}(-k) f(k)] \in L^2(\mathbb{R})$, and, since $f(k) \neq 0$ on $\mathbb{R}$ and $f(\infty) = 1$, it follows that $g \in L^2(\mathbb{R})$. The inclusion $[\dot{f}(k) f(-k) - \dot{f}(-k) f(k)] \in L^2(\mathbb{R})$ follows from (2.40)-(2.42) and (2.46)-(2.47).

The converse step

$$H(t) \Rightarrow f(k) \tag{2.52}$$

is also done by formula (1.17): Fourier inversion gives $|f(k)|^2 = f(k) f(-k)$, and factorization yields the unique $f(k)$, since $f(k)$ does not vanish in $\mathbb{C}_+$ and tends to 1 at infinity.

Step 3. $H \Rightarrow \Gamma_x(s, 0) \Rightarrow \Gamma_{2x}(2x, 0)$.

This step is done by solving equation (1.6). By Theorem 1.3 equation (1.6) is uniquely solvable since condition (1.7) is assumed. Formula (1.17) holds and the known properties of the Jost function (1.4) are used: $f(k) \to 1$ as $k \to \pm\infty$, $f(k) \neq 0$ for $k \neq 0$, $k \in \mathbb{R}$, $f(0) \neq 0$ since $\mathrm{ind}_{\mathbb{R}} S(k) = 0$.

The converse step $\Gamma_x(s, 0) \Rightarrow H(t)$ is done by formula (1.6"). The converse step

$$\Gamma_{2x}(2x, 0) \Rightarrow \Gamma_x(s, 0) \tag{2.53}$$

constitutes the essence of the inversion method.

This step is done as follows:

$$\Gamma_{2x}(2x,0) \overset{(1.18)}{\Rightarrow} a(x) \overset{(2.17)-(2.18)}{\Rightarrow} E(x,k) \overset{(1.11)}{\Rightarrow} \Gamma_x(s,0). \tag{2.54}$$

Given $a(x)$, system (2.17)-(2.18) is uniquely solvable for $E(x,k)$.

Note that the step $q(x) \Rightarrow f(k)$ can be done by solving the uniquely solvable integral equation (see [**?**]):

$$f(x,k) = e^{ikx} + \int_x^\infty \frac{\sin[k(y-x)]}{k} q(y) f(y,k) dy \tag{2.55}$$

with $q \in L_{1,1}(\mathbb{R}_+)$, and then calculating $f(k) = f(0,k)$.

Step 4. $a(x) := 2\Gamma_{2x}(2x,0) \Rightarrow q(x)$.

This step is done by formula (1.19). The converse step

$$q(x) \Rightarrow a(x)$$

can be done by solving the Riccati problem (1.19) for $a(x)$ given $q(x)$ and the initial condition $2H(0)$. Given $q(x)$, one can find $2H(0)$ as follows: one finds $f(x,k)$ by solving equation (2.55), which is uniquely solvable if $q \in L_{1,1}(\mathbb{R}_+)$, then one gets $f(k) := f(0,k)$, and then calculates $2H(0)$ using formula (2.49) with $t = 0$:

$$2H(0) = \frac{1}{\pi} \int_{-\infty}^\infty \left(\frac{1}{|f(k)|^2} - 1 \right) dk.$$

Proof of Theorem 1.1. If (1.20)-(1.22) hold, then, as has been proved in [**?**] (and earlier in a different form in [**?**]), there is a unique $q(x) \in L_{1,1}(\mathbb{R}_+)$ which generates the given S-matrix $S(k)$.

*It is not proved in [**?**] that $q(x)$ defined in (1.19) (and obtained as a final result of steps 1) – 4)) generates the scattering matrix $S(k)$ with which we started the inversion.*

Let us now prove this. We have already discussed the following diagram:

$$S(k) \underset{(1.16)}{\overset{(2.38)}{\Leftrightarrow}} f(k) \overset{(1.17)}{\Leftrightarrow} H(t) \overset{(1.6)}{\Leftrightarrow} \Gamma_x(s,0) \Rightarrow \Gamma_{2x}(2x,0) \overset{(1.18)}{\Leftrightarrow} a(x) \overset{(1.19)}{\Leftrightarrow} q(x). \tag{2.56}$$

To close this diagram and therefore establish the basic one-to-one correspondence

$$S(k) \Leftrightarrow q(x), \tag{2.57}$$

one needs to prove

$$\Gamma_{2x}(2x,0) \Rightarrow \Gamma_x(s,0).$$

This is done by the scheme (2.54).

Note that the step $q(x) \Rightarrow a(x)$ requires solving Riccati equation (1.19) with the boundary condition $a(0) = 2H(0)$. Existence of the solution to this problem on all of $\mathbb{R}_+$ is guaranteed by the assumptions (1.20)-(1.22). The fact that these assumptions imply $q(x) \in L_{1,1}(\mathbb{R}_+)$ is proved in [**?**] and [**?**]. Theorem 1.1 is proved. □

Uniqueness theorems for the inverse scattering problem are not given in [**?**], [**?**]. They can be found in [**?**]-[**?**].

Remark 2.1. *From our analysis one gets the following result:*

Proposition 2.1. *If $q(x) \in L_{1,1}(\mathbb{R}_+)$ and has no bounds states and no resonance at zero, then Riccati equation (1.19) with the initial condition (1.18) has the solution $a(x)$ defined for all $x \in \mathbb{R}_+$.*

3 Numerical aspects of the Krein inversion procedure.

The main step in this procedure from the numerical viewpoint is to solve equation (1.6) for all $x > 0$ and all $0 < s < x$, which are the parameters in equation (1.6).

Since equation (1.6) is an equation with the convolution kernel, its numerical solution involves inversion of a Toeplitz matrix, which is a well developed area of numerical analysis. Moreover, such an inversion requires much less computer memory and time than the inversion based on the Gel'fand-Levitan or Marchenko methods. This is the main advantage of Krein's inversion method.

This method may become even more attractive if it is combined with the Marchenko method. In the Marchenko method the equation to be solved is ([**?**], [**?**]):

$$A(x,y) + F(x+y) + \int_x^\infty A(x,s)F(s+y)ds = 0, \quad y \geq x \geq 0, \tag{3.1}$$

where $F(x)$ is defined in (1.23) and is known if $S(k)$ is known, the kernel $A(x,y)$ is to be found from (3.1) and if $A(x,y)$ is found then the potential is recovered by the formula:

$$q(x) = -2\frac{dA(x,x)}{dx}. \tag{3.2}$$

Equation (3.1) can be written in operator form:

$$(I + F_x)A = -F. \tag{3.3}$$

The operator F_x is a contraction mapping in the Banach space $L^1(x,\infty)$ for $x > 0$. The operator H_x in (1.6) is a contraction mapping in $L^\infty(0,x)$ for $0 < x < x_0$, where x_0 is chosen to that

$$\int_0^{x_0} |H(t-u)|du < 1. \tag{3.4}$$

Therefore it seems reasonable from the numerical point of view to use the following approach:

1. Given $S(k)$, calculate $f(k)$ and $H(t)$ as explained in Steps 1 and 2, and also $F(x)$ by formula (1.23).

2. Solve by iterations equation (1.6) for $x < x < x_0$, where x_0 is chosen so that the iteration method for solving (1.6) converges rapidly. Then find $q(x)$ as explained in Step 4.

3. Solve equation (3.1) for $x > x_0$ by iterations. Find $q(x)$ for $x > x_0$ by formula (3.2).

4 Discussion of the ISP when the bound states are present.

If the given data are (1.1), then one defines

$$w(k) = \prod_{j=1}^{J} \frac{k - ik_j}{k + ik_j} \quad \text{if} \quad \text{ind}_{\mathbb{R}} S(x) = -2J \tag{4.1}$$

and

$$W(k) = \frac{k}{k + i\gamma} w(k) \quad \text{if} \quad \text{ind}_R S(k) = -2J - 1, \tag{4.2}$$

where $\gamma > 0$ is arbitrary, and is chosen so that $\gamma \neq k_j$, $1 \leq j \leq J$.

Then one defines

$$S_1(k) := S(k) w^2(k) \quad \text{if} \quad \text{ind}_{\mathbb{R}} S = -2J \tag{4.3}$$

or

$$S_1(k) := S(k) W^2(k) \quad \text{if} \quad \text{ind}_{\mathbb{R}} S = -2J - 1. \tag{4.4}$$

Since $\text{ind}_{\mathbb{R}} w^2(k) = 2J$ and $\text{ind}_{\mathbb{R}} W^2(k) = 2J + 1$, one has

$$\text{ind}_{\mathbb{R}} S_1(k) = 0. \tag{4.5}$$

The theory of section 2 applies to $S_1(k)$ and yields $q_1(x)$. From $q_1(x)$ one gets $q(x)$ by adding bound states $-k_j^2$ and norming constants s_j using the known procedure (e.g. see [**?**]).

5 Relation between Krein's and GL's methods.

The GL (Gel'fand-Levitan) method in the absence of bound states consists of the following steps (see [**?**], for example):

<u>Step 1.</u> Given $f(k)$, the Jost function, find

$$\begin{aligned} L(x, y) &:= \frac{2}{\pi} \int_0^\infty dk\, k^2 \left(\frac{1}{|f(k)|^2} - 1 \right) \frac{\sin kx}{k} \frac{\sin ky}{k} \\ &= \frac{1}{\pi} \int_0^\infty dk \left(|f(k)|^{-2} - 1 \right) \left(\cos[k(x - y)] - \cos[k(x + y)] \right) \\ &:= M(x - y) - M(x + y), \end{aligned} \tag{5.1}$$

where

$$M(x) := \frac{1}{\pi} \int_0^\infty dk \left(|f(k)|^{-2} - 1 \right) \cos(kx). \tag{5.2}$$

Step 2. Solve the integral equation for $K(x, y)$:

$$K(x, y) + L(x, y) + \int_0^x K(x, s) L(s, y) ds = 0, \quad 0 \le y \le x. \tag{5.3}$$

Step 3. Find

$$q(x) = 2 \frac{dK(x, x)}{dx}. \tag{5.4}$$

Krein's function (see (1.17)) can be written as follows:

$$H(t) = \frac{1}{2\pi} \int_{-\infty}^\infty \left(|f(k)|^{-2} - 1 \right) e^{-ikt} dk = \frac{1}{\pi} \int_0^\infty \left(|f(k)|^{-2} - 1 \right) \cos(kt) dk. \tag{5.5}$$

Thus, the relation between the two methods is given by the formula:

$$M(x) = H(x). \tag{5.6}$$

In fact, the GL method deals with the inversion of the spectral foundation $d\rho$ of the operator $-\frac{d^2}{dx^2} + q(x)$ defined in $L^2(\mathbb{R}_+)$ by the Dirichlet boundary condition at $x = 0$. However, if $\text{ind}_{\mathbb{R}} S(k) = 0$ (in this case there are no bound states and no resonance at $k = 0$), then (see e.g. [**?**]):

$$d\rho(\lambda) = \begin{cases} \frac{2k^2 dk}{\pi |f(k)|^2}, & \lambda > 0, \quad \lambda = k^2, \\ 0, & \lambda < 0, \end{cases}$$

so $d\rho(\lambda)$ in this case is uniquely defined by $f(k)$, $k \ge 0$.

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