INVERSE PROBLEM ON THE LINE WITHOUT PHASE INFORMATION

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Abstract: The one-dimensional Schrödinger equation is considered for real potentials that are integrable, have finite first moment, and contain no bound states. The recovery of a potential with support in a right half-line is studied in terms of the scattering data consisting of the magnitude of the reflection coefficient, a known potential placed to the left of the unknown potential, and the magnitude of the reflection coefficient of the combined potential. Several kinds of methods are described for retrieval of the reflection coefficient corresponding to the unknown potential. Some illustrative examples are provided.

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1. INTRODUCTION

Consider the one-dimensional Schrödinger equation

$$\psi''(k,x) + k^2\psi(k,x) = V(x)\,\psi(k,x), \qquad x \in \mathbf{R}, \tag{1.1}$$

where the potential V is real valued and belongs to $L^1_1(\mathbf{R})$, i.e. $\int_{-\infty}^{\infty} dx\,(1+|x|)\,|V(x)|$ is finite. The scattering states of (1.1) correspond to its solutions behaving like e^{ikx} or e^{-ikx} as $x \to \pm\infty$. Among such solutions are the Jost solution from the left $f_l(k,x)$ and the Jost solution from the right $f_r(k,x)$ satisfying

$$f_l(k,x) = \begin{cases} e^{ikx} + o(1), & x \to +\infty, \\ \dfrac{1}{T(k)}e^{ikx} + \dfrac{L(k)}{T(k)}e^{-ikx} + o(1), & x \to -\infty, \end{cases} \tag{1.2}$$

$$f_r(k,x) = \begin{cases} \dfrac{1}{T(k)}e^{-ikx} + \dfrac{R(k)}{T(k)}e^{ikx} + o(1), & x \to +\infty, \\ e^{-ikx} + o(1), & x \to -\infty, \end{cases}$$

where T is the transmission coefficient, and R and L are the reflection coefficients from the right and from the left, respectively. The scattering matrix associated with V is given by

$$\mathbf{S}(k) = \begin{bmatrix} T(k) & R(k) \\ L(k) & T(k) \end{bmatrix}, \tag{1.3}$$

and it satisfies

$$\mathbf{S}(-k) = \mathbf{S}(k)^*, \qquad k \in \mathbf{R}, \tag{1.4}$$

where the asterisk denotes complex conjugation. The bound states correspond to the square-integrable solutions of (1.1), and such states occur only at certain negative k^2 values known as bound-state energies. The recovery of V using a reflection coefficient, the bound-state energies, and the so-called norming constants constitutes the inverse scattering problem, and its solution can be obtained by using one of the available inversion methods

[Fa64,DT79,Ma86,CS89,Sa93]. When there are no bound states, a reflection coefficient uniquely determines the potential.

In this paper we consider the inverse scattering problem when the data consist of the reflectivity $r = |L| = |R|$, that is, the magnitude of the reflection coefficients. Unless otherwise stated, we assume that no bound states exist, so that by the above discussion the unknown potential can be determined provided we can find the phase of L or R. Such problems are motivated by interesting applications in neutron and x-ray scattering studies of surface and interface structures, see e.g. [FR91,FY96,ZC95].

It is well known that in general one cannot uniquely determine the potential from reflectivity data, although uniqueness is known for certain special classes of potentials, see e.g. [Cl93,KST95,BM96]. Hence, we will augment our scattering data by including also the reflectivity corresponding to the situation in which a known nontrivial potential is placed to the left of the unknown potential (Figure 1). Use of this kind of data has been considered by several researchers recently (e.g. [KS92,MB96,HWAF95,HWSAF96]), so let us explain right away how the approach taken here relates to these other works.

Consider a potential $V(x) = V_1(x) + V_2(x)$ where $V_1(x) = 0$ for $x > a$ and $V_2(x) = 0$ for $x < a$, for some finite a. From our point of view, V_2 is the unknown potential we wish to determine, and V_1 represents a known layer "in front of" V_2, i.e. we are measuring the reflected intensity of waves incident from the left. For any choice of V_1 we thus assume that $|L|$ can be measured for $0 < k < +\infty$, where L is the left reflection coefficient implicitly defined in (1.2). Thus, data for the inverse scattering problem consist of $\{|L|, V_1\}$, or equivalently $\{|L|, \mathbf{S}_1\}$, where $\mathbf{S}_1$ is the scattering matrix for V_1 and is defined as in (1.3). (We assume that V_1 also has no bound states.) In general we may assume that such data are available for several different choices of V_1.

In [KS92] it was shown, under somewhat restrictive conditions on the potential, that the data $\{|L|, V_1\}$, for one choice of V_1 satisfying a nondegeneracy condition, determine V_2 uniquely. On the other hand in [MB96,HWAF95,HWSAF96] it was shown that $\{|L|, V_1\}$ for three different choices of V_1 determines V_2 under less restrictive conditions.

There is a further distinction between the method of [KS92] (the one-measurement method) and that of [MB96,HWAF95,HWSAF96] (the three-measurement method) which we wish to emphasize, namely the former is a *global* method while the latter is *local*. By a global method we mean that one recovers the phase of L_2 for all k given the scattering data for all k, while in the local method one can recover the phase of L_2 at any one fixed value of k from the scattering data at the same fixed value of k. For most purposes a local method will be preferable, since unavoidable inaccuracies at high or low frequencies will not affect the computed solution at other frequencies. The local method will also tend to be easier from a computational point of view. On the other hand, with a global method we may be able to get more accurate phase information at high and low frequencies than could be obtained with a purely local method.

The present paper fills in the gap between the one- and three-measurement techniques cited above, namely we consider the recovery of V_2 from two reflectivity measurements. We will generally assume that one of the two measurements corresponds to $V_1(x) = 0$, in which case the reflectivity measurement is just $|L_2|$ itself, where L_2 is the left reflection coefficient for V_2. However the method could be easily adapted to the case of two nonzero choices of V_1, as shown at the end of Section 2.

We will derive two different methods for determination of the phase of L_2, one of the global type and one of the local type. The global method, discussed in Section 2, is in principle somewhat easier to use than the global method of [KS92], while the local method, discussed in Section 3, is somewhat more complicated than its counterpart in [MB96,HWAF95,HWSAF96]. Nevertheless, it is probably not possible to assert that any one of these methods is always better than the others, but rather it will depend on specific circumstances. The methods will be illustrated with analytical and numerical examples.

2. GLOBAL TWO-LAYER METHOD

In this section we consider the recovery of V_2 by using two reflectivity measurements at each k for $k \in [0, +\infty)$. This will be done by constructing L_2. The construction of L_2 requires the construction of an intermediate function for all $k \in \mathbf{R}$, and hence the method described here is a global one. The intermediate function can be chosen as F defined in (2.5), or alternatively the transmission coefficients corresponding to the two measured reflectivities.

Let $\mathbf{S}_1$, $\mathbf{S}_2$, and $\mathbf{S}$ be the scattering matrices corresponding to the potentials V_1, V_2, and V, respectively. Corresponding to V_j with $j = 1, 2$, as in (1.3), we have the transmission coefficient T_j and the reflection coefficients R_j and L_j, from the right and left, respectively, forming the scattering matrix:

$$\mathbf{S}_j(k) = \begin{bmatrix} T_j(k) & R_j(k) \\ L_j(k) & T_j(k) \end{bmatrix}, \qquad j = 1, 2.$$

Let us define the transition matrix associated with $\mathbf{S}(k)$:

$$\Lambda(k) = \begin{bmatrix} \dfrac{1}{T(k)} & -\dfrac{R(k)}{T(k)} \\ \dfrac{L(k)}{T(k)} & \dfrac{1}{T(k)^*} \end{bmatrix} = \begin{bmatrix} \dfrac{1}{T(k)} & \dfrac{L(k)^*}{T(k)^*} \\ \dfrac{L(k)}{T(k)} & \dfrac{1}{T(k)^*} \end{bmatrix} = \begin{bmatrix} \dfrac{1}{T(k)} & -\dfrac{R(k)}{T(k)} \\ -\dfrac{R(k)^*}{T(k)^*} & \dfrac{1}{T(k)^*} \end{bmatrix}.$$

Similarly, let Λ_1 and Λ_2 be the transition matrices corresponding to $\mathbf{S}_1$ and $\mathbf{S}_2$. It is known [Ak92] that

$$\Lambda(k) = \Lambda_1(k)\,\Lambda_2(k). \tag{2.1}$$

Using the $(1,1)$-entry in the matrix product in (2.1), we get

$$\frac{1}{T(k)} = \frac{1}{T_1(k)\,T_2(k)} - \frac{R_1(k)}{T_1(k)}\frac{L_2(k)}{T_2(k)}, \tag{2.2}$$

from which we obtain

$$L_2(k) = \frac{1}{R_1(k)} \left[1 - \frac{T_1(k)\, T_2(k)}{T(k)} \right]. \tag{2.3}$$

Thus, knowing $\{R_1, T_1, T_2, T\}$ we can construct L_2. By an analytic continuation argument it is not hard to see that $R_1(k)$ cannot vanish identically on any interval of the real axis, unless $V_1 \equiv 0$. More generally, results in the theory of Hardy spaces [DM76] imply that the set of points at which $R_1(k) = 0$ is of measure zero, and so (2.3) still determines L_2 almost everywhere, which is sufficient for the purpose of recovering V_2 via inverse scattering theory.

If V has no bound states, then T is determined [Fa64,DT79,CS89] by $|L|$ given for $k \in [0, +\infty)$. If neither V_1 nor V_2 have any bound states, then V cannot have any bound states either; this is because the number of bound states for V cannot exceed the total number of bound states for V_1 and V_2. In this case, using $\{R_1, |L_2|, |L|\}$ given for $k \in [0, +\infty)$, with the help of

$$|T_1(k)|^2 = 1 - |R_1(k)|^2, \qquad |T_2(k)|^2 = 1 - |L_2(k)|^2, \qquad |T(k)|^2 = 1 - |L(k)|^2, \tag{2.4}$$

one can construct $\{T_1, T_2, T\}$ for $k \in \overline{\mathbf{C}^+}$, and hence with the help of (2.3) one can recover L_2 using $\{R_1, |L_2|, |L|\}$ for $k \in [0, +\infty)$. We use $\mathbf{C}^+$ to denote the upper-half complex plane and $\overline{\mathbf{C}^+}$ for its closure. In summary, we have the following result.

Theorem 2.1 Assume $V \in L^1_1(\mathbf{R})$, let V_1 and V_2 be its fragments with supports in $(-\infty, a]$ and $[a, +\infty)$, respectively for some finite a, and suppose V_1 is nontrivial. If V_1 and V_2 are free of bound states, then L_2 for $k \in \overline{\mathbf{C}^+}$ is uniquely determined by $\{R_1, |L_2|, |L|\}$ given for $k \in [0, +\infty)$.

Although the construction of the transmission coefficient in terms of the corresponding reflectivity is straightforward mathematically, it may not be so easy as far as practical computations are concerned. Next, we will describe a simpler global procedure to recover

L_2 from $\{R_1, |L_2|, |L|\}$, where one does not need to construct $\{T_1, T_2, T\}$. This method requires the construction of the intermediate function F defined as

(2.5) $$F(k) = 1 - R_1(k)\, L_2(k), \qquad k \in \mathbf{R}.$$

Theorem 2.2 Under the conditions stated in Theorem 2.1, the quantity F defined in (2.5) is uniquely determined in $\overline{\mathbf{C}^+}$ in terms of $\{|R_1|, |L_2|, |L|\}$ given for $k \in [0, +\infty)$.

PROOF: From (2.2) we see that

(2.6) $$F(k) = \frac{T_1(k)\, T_2(k)}{T(k)}.$$

Because of (1.4), we have $F(-k) = F(k)^*$ for real values of k. It is known that T_1, T_2, and T do not have any zeros in $\overline{\mathbf{C}^+} \setminus \{0\}$. Since V_1 and V_2 are assumed not to contain any bound states, it follows that T_1, T_2, and T can be continued analytically from the real axis to $\mathbf{C}^+$ and are continuous in $\overline{\mathbf{C}^+}$. Hence, as seen from (2.6), F can be continued analytically from the real axis to $\mathbf{C}^+$, and it is continuous in $\overline{\mathbf{C}^+}$ and nonzero in $\overline{\mathbf{C}^+} \setminus \{0\}$. Moreover, we have

(2.7) $$F(k) = 1 + O(1/k^2), \qquad k \to \infty \text{ in } \overline{\mathbf{C}^+},$$

which is obtained by using (2.5) and the fact that V_1 and V_2 each have support in a half-line. Hence, one can construct F in $\overline{\mathbf{C}^+}$ by using only its magnitude $|F|$ on the real axis or simply on $[0, +\infty)$ because of $F(-k) = F(k)^*$ for $k \in \mathbf{R}$. This recovery can be achieved by solving a Riemann-Hilbert problem. From (2.4) and (2.6), we have

(2.8) $$F(k)\, F(-k) = \frac{[1 - |R_1(k)|^2][1 - |L_2(k)|^2]}{1 - |L(k)|^2}, \qquad k \in \mathbf{R}.$$

We can express $F(k)$ explicitly as

(2.9)
$$F(k) = \exp\left\{ \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{dz}{z - k - i0} \log\left(\frac{[1 - |R_1(z)|^2][1 - |L_2(z)|^2]}{1 - |L(z)|^2} \right) \right\}, \qquad k \in \overline{\mathbf{C}^+}.$$

One can also obtain F by solving the Riemann-Hilbert problem (2.8) using other methods such as Wiener-Hopf factorization or by solving a related singular integral equation [Ga66,Mu46]. ∎

Having constructed F in terms of $\{|R_1, ||L_2|, |L|\}$ as indicated in the above proof, one can recover L_2 by using

$$L_2(k) = \frac{1 - F(k)}{R_1(k)}, \tag{2.10}$$

which is obtained from (2.5). Thus the recovery of L_2 is accomplished without constructing $\{T_1, T_2, T\}$.

As far as the recovery of L_2 is concerned, the method implicit in Theorem 2.2 is better than that in Theorem 2.1. In the former only one Hilbert transform is needed instead of two needed in the latter. In the former method one does not need T_1. Furthermore, although $T - 1$ and $T_2 - 1$ decay as $O(1/k)$ as $k \to \infty$, as seen from (2.7), $F - 1$ decays more rapidly, and hence the numerical construction of the Hilbert transform may be more accurate in the former method.

As a final remark we note that one can also obtain L_2 by measuring one at a time the reflectivity of the combined potential with two known, nontrivial layers. This can be seen as follows. Let V_1 and $\tilde{V}_1$ be two known potentials with support contained in $(-\infty, a]$ with scattering matrices $\mathbf{S}_1$ and $\tilde{\mathbf{S}}_1$, respectively; let Λ_1 and $\tilde{\Lambda}_1$ denote the corresponding transition matrices, respectively. Let $V(x) = V_1(x) + V_2(x)$ and $\tilde{V}(x) = \tilde{V}_1(x) + V_2(x)$. As in (2.1) we have

$$\Lambda(k) = \Lambda_1(k)\,\Lambda_2(k), \qquad \tilde{\Lambda}(k) = \tilde{\Lambda}_1(k)\,\Lambda_2(k). \tag{2.11}$$

The $(1,1)$ entries of the matrices in (2.11) give us (2.2) and

$$\frac{1}{\tilde{T}(k)} = \frac{1}{\tilde{T}_1(k)\,T_2(k)} - \frac{\tilde{R}_1(k)}{\tilde{T}_1(k)}\frac{L_2(k)}{T_2(k)}. \tag{2.12}$$

Eliminating $T_2(k)$ from (2.2) and (2.12), we obtain

$$L_2(k) = \frac{\tilde{T}_1(k)\,T(k) - T_1(k)\,\tilde{T}(k)}{R_1(k)\,\tilde{T}_1(k)\,T(k) - \tilde{R}_1(k)\,T_1(k)\,\tilde{T}(k)}.$$

Thus, one can construct L_2 using $\{V_1, \tilde{V}_1, T, \tilde{T}\}$. In case neither V nor $\tilde{V}$ have any bound states, we can conclude that V_2 for $x \in \mathbf{R}$ can be constructed using $\{V_1, \tilde{V}_1, |L|, |\tilde{L}|\}$ for $k \in [0, +\infty)$.

Next we illustrate the recovery of V_2 in terms of $\{R_1, |L_2|, |L|\}$ by the global method outlined in this section.

Example 2.3 Let us use the following data:

$$|L_2(k)|^2 = \frac{9}{4k^4 + 4k^2 + 9}, \quad |L(k)|^2 = \frac{4k^2 + 289}{16k^6 + 20k^4 + 8k^2 + 289}, \tag{2.13}$$

$$R_1(k) = \frac{2}{2k^2 + 3ik - 2}, \tag{2.14}$$

where R_1 corresponds to

$$V_1(x) = \frac{4e^{-x}}{(2e^{-x} - 1)^2}\,\theta(-x),$$

with $\theta(x)$ denoting the Heaviside function. We assume that V_2 has no bound states. Using $\{|R_1|^2, |L_2|^2, |L|^2\}$, we first write (2.8) as

$$F(k)\,F(-k) = \frac{k^2(16k^6 + 20k^4 + 8k^2 + 289)}{(4k^4 + 4k^2 + 9)(4k^4 + k^2 + 4)},$$

from which, through factorization, we get

$$F(k) = \frac{k(4k^3 + 14ik^2 - 22k - 17i)}{(2k^2 + 3ik - 2)(2k^2 + 4ik - 3)}.$$

Thus we construct L_2 using (2.10) as

$$L_2(k) = \frac{3}{2k^2 + 4ik - 3}, \tag{2.15}$$

which corresponds to

$$V_2(x) = \frac{24e^{2x}}{(3e^{2x}-1)^2}\,\theta(x). \tag{2.16}$$

3. LOCAL TWO-LAYER METHOD

In this section we consider the construction of L_2 at any one fixed k value in terms of $\{R_1(k), |L_2(k)|, |L(k)|\}$ at that k value.

Suppose we know the reflectivity L at a particular k value but not for all $k \in \mathbf{R}$. Then we can only obtain $|T|$ at this particular k value but not T itself. In other words, the analyticity of T in $\mathbf{C}^+$, its continuity in $\overline{\mathbf{C}^+}$, its small-k and large-k asymptotics cannot be used to construct the transmission coefficient at a single point from knowledge of its magnitude at that point.

It is known [HWAF95,HWSAF96] that there are in general two candidates for L_2 corresponding to $\{R_1, |L_2|, |L|\}$ at a particular k, and these two candidates can be obtained as the intersection of two circles on the complex plane. By using a different reflection coefficient $\tilde{R}_1$, one obtains L_2 as the intersection of three circles in the plane [HWAF95,HWSAF96].

In this section we study the construction of L_2 by using the intersection of a circle and one line in the plane. We analyze the two different candidates for L_2 constructed from the intersection of a circle and a line, show how these two are related to each other, and indicate how we can discard one of these in favor of the other.

Let us separate the real and imaginary parts of L_2 and R_1 :

$$L_2(k) = \alpha(k) + i\beta(k), \qquad R_1(k) = \gamma(k) + i\epsilon(k). \tag{3.1}$$

For simplicity, let us drop the arguments and simply write α instead of $\alpha(k)$; let us also use the same convention for β, γ, ϵ. We have

$$\alpha^2 + \beta^2 = |L_2|^2, \tag{3.2}$$

which represents a circle centered at the origin with radius $|L_2|$ in the (α, β)-plane. From (2.3) we get

$$1 - R_1(k)\, L_2(k) = \frac{T_1(k)\, T_2(k)}{T(k)}. \tag{3.3}$$

We would like to construct L_2 at a particular k value by using $\{R_1, |L_2|, |L|\}$ at this k value. Equivalently, because of (2.6) we know $\{R_1, |T_1|, |T_2|, |L_2|, |T|\}$ at a particular k value and we are interested in constructing L_2. Our data do not allow us to use (3.3), but by taking the absolute value of both sides of (3.3) and using (2.6), we get the real part of $R_1\, L_2$ as

$$\text{Re}\,\{R_1(k)\, L_2(k)\} = A(k), \tag{3.4}$$

where we have defined

$$A(k) = \frac{1}{2}\left[1 + |R_1(k)|^2\, |L_2(k)|^2 - \frac{[1-|R_1(k)|^2][1-|L_2(k)|^2]}{1-|L(k)|^2}\right]. \tag{3.5}$$

We can write (3.4) as

$$\gamma\alpha - \epsilon\beta = A, \tag{3.6}$$

which is the equation of a line in the (α, β)-plane. The two points of intersection of the circle (3.2) and the line (3.6) is given by

$$\alpha = \frac{2\gamma A + \epsilon\, Z^{1/2}}{2|R_1|^2}, \qquad \beta = \frac{\gamma\alpha - A}{\epsilon}, \tag{3.7}$$

where the square-root function in (3.7) is double-valued and we have defined

$$Z(k) = 4\,|R_1(k)|^2\, |L_2(k)|^2 - 4A(k)^2. \tag{3.8}$$

Theorem 3.1 The quantity Z defined in (3.8) is a nonnegative function of k on $[0,+\infty)$. We have $Z(k_0)=0$ at some positive k_0 if and only if $[R_1(k_0)\,L_2(k_0)]$ is real.

PROOF: Using the triangle inequality in (3.3) we get

$$1-|R_1|\,|L_2|\le\left|\frac{T_1\,T_2}{T}\right|\le 1+|R_1|\,|L_2|, \tag{3.9}$$

and hence

$$\left|\frac{T_1\,T_2}{T}\right|^2-[1-|R_1|\,|L_2|]^2\ge 0,\qquad [1+|R_1|\,|L_2|]^2-\left|\frac{T_1\,T_2}{T}\right|^2\ge 0.$$

Let us write (3.8) in the factored form as

$$Z=[2\,|R_1|\,|L_2|-2A]\,[2\,|R_1|\,|L_2|+2A]\,. \tag{3.10}$$

Using (3.5) in (3.10), after some simplification, we get

$$Z=\left[\left|\frac{T_1\,T_2}{T}\right|^2-[1-|R_1|\,|L_2|]^2\right]\left[[1+|R_1|\,|L_2|]^2-\left|\frac{T_1\,T_2}{T}\right|^2\right], \tag{3.11}$$

or equivalently $Z=B_1\,B_2\,B_3\,B_4$, where we have defined

$$B_1=\left|\frac{T_1\,T_2}{T}\right|-1+|R_1|\,|L_2|,\qquad B_2=\left|\frac{T_1\,T_2}{T}\right|+1-|R_1|\,|L_2|, \tag{3.12}$$

$$B_3=-\left|\frac{T_1\,T_2}{T}\right|+1+|R_1|\,|L_2|,\qquad B_4=\left|\frac{T_1\,T_2}{T}\right|+1+|R_1|\,|L_2|. \tag{3.13}$$

Using (3.9) in (3.12) and (3.13) we obtain

$$0\le B_1\le 2\,|R_1|\,|L_2|,\qquad 2[1-|R_1|\,|L_2|]\le B_2\le 2,$$

$$0\le B_3\le 2\,|R_1|\,|L_2|,\qquad 2\le B_4\le 2\,[1+|R_1|\,|L_2|],$$

and hence Z is a nonnegative function of k, and the only zeros of Z in $(0,+\infty)$ come from B_1 or B_3; note that B_2 and B_4 are strictly positive in $(0,+\infty)$. From (3.3), (3.12), and (3.13) we see that $B_1\, B_3 = 0$ at some positive k value if and only if $|1 - R_1\, L_2| = 1 \pm |R_1\, L_2|$ at that k value. Thus, $Z(k_0) = 0$ at some positive k_0 if and only if $\text{Im}\,\{R_1(k_0)\, L_2(k_0)\} = 0$. ∎

Since Z is a nonnegative function of k, the double-valued function $Z^{1/2}$ is also real valued. Thus, L_2 is determined pointwise by (3.7) up to the uncertainty in the sign of $Z^{1/2}$. If we can decide what branch of the square-root function in (3.7) leads to L_2, we can uniquely construct L_2 at a given k value by using $\{R_1, |L_2|, |L|\}$ at this k value. Later in the section we will show which branch of $Z^{1/2}$ gives us the "correct" L_2.

Theorem 3.2 The two $\alpha(k) + i\beta(k)$ formed from the two values given in (3.7) are equal to $L_2(k)$ and $R_1(k)^*\, L_2(k)^*/R_1(k)$, respectively. Consequently, if these two (α, β) values in (3.7) are used in (2.5), we obtain $1 - R_1(k)\, L_2(k)$ and $1 - R_1(k)^*\, L_2(k)^*$, respectively.

PROOF: From (2.5), (3.4), and (3.5) it is clear that at each particular k value, the real part of F is determined pointwise by $\{|R_1|, |L_2|, |L|\}$:

$$\text{Re}\,\{F(k)\} = \frac{1}{2}\left[1 - |R_1(k)|^2\,|L_2(k)|^2 + \frac{[1 - |R_1(k)|^2][1 - |L_2(k)|^2]}{1 - |L(k)|^2}\right]. \tag{3.14}$$

Now let us show that the double-valued pair (α, β) given in (3.7) determine the imaginary part of F up to a sign factor. Using (3.1) in (2.5) we get

$$\text{Im}\,\{F(k)\} = -\epsilon\alpha - \gamma\beta. \tag{3.15}$$

If the two (α, β) values given in (3.7) are used in (3.15), using $\gamma^2 + \epsilon^2 = |R_1(k)|^2$, we can simplify (3.15) to

$$[\text{Im}\,\{F(k)\}]^2 = \frac{1}{4}\, Z. \tag{3.16}$$

Hence the two L_2 values obtained by using (3.7) at a particular k value determine F up to a sign in its imaginary part. In other words, one branch of the square-root function leads to F that can be extended analytically to $\mathbf{C}^+$, and the other branch leads to the complex conjugate of that function. When used on the right-hand side of (2.5), the former gives us $L_2(k)$ that is associated with V_2, and the latter gives us $R_1(k)^* \, L_2(k)^*/R_1(k)$, which cannot be extended analytically to $\mathbf{C}^+$ and hence cannot correspond to a potential without bound states and with support on a right half-line. ∎

As seen from (2.5), since $0 \le |R_1 \, L_2| < 1$ on $(0, +\infty)$, it follows that $\text{Re}\,\{F(k)\} > 0$ on $(0, +\infty)$ and the graph of the curve $k \mapsto F$ on $(0, +\infty)$ is continuous and confined to the right-half of the complex plane and converges to $1 + 0i$. as $k \to +\infty$.

A potential is generic if its reflectivity at $k = 0$ is equal to one; otherwise, the potential is exceptional [CS89]. If V_1 and V_2 are free of bound states and they are both generic, then the curve representing F on the complex plane approaches 0 as $k \to 0+$ along the negative imaginary axis [AKV97]. Using Theorem 3.2, we can thus conclude that the "correct" L_2 value causes $\text{Im}\,\{F(k)\}$ to approach zero through negative values as $k \to 0+$. We will not deal with the case when at least one of V_1 and V_2 is exceptional because in that case, the sign of $\text{Im}\,\{F(k)\}$ cannot be determined easily unless we have more information about V_2. Moreover, a small perturbation of an exceptional potential may change the number of bound states and in this paper we avoid potentials with bound states. For further information we refer the reader to [AKV97] and the references therein.

Let us analyze the zeros of Z on $(0, +\infty)$ more closely. As we have seen in Theorem 3.1, $Z(k_0) = 0$ for some $k_0 \in (0, +\infty)$ if and only if $\text{Im}\,\{F(k_0)\} = 0$. Since $F(k)$ is continuous at k_0, the tangent line to the graph of $k \mapsto F$ must change continuously at k_0, and hence we can determine if $\text{Im}\,\{F(k)\}$ changes sign at k_0 by analyzing the graph of $k \mapsto |\sqrt{Z(k)}|$ near k_0. For example, if k_0 corresponds to an odd-order zero of $|\sqrt{Z(k)}|$ then the sign of $\text{Im}\,\{F(k)\}$ must change at k_0, and if k_0 has even order then the sign of $\text{Im}\,\{F(k)\}$ must not change at k_0. Let us define $\sqrt{Z(k)}$ as the single-valued branch of $[Z(k)]^{1/2}$ whose argument changes continuously and such that $\sqrt{Z(k)}$ remains nonnegative as $k \to 0+$.

Let $0 < k_1 < k_2 < k_3 < \cdots$ be the ordered zeros of Z given in (3.11). Then $\sqrt{Z(k)}$ and $|\sqrt{Z(k)}|$ coincide in $[0, k_1]$; they either differ by a sign in $[k_1, k_2]$ or they coincide, and in the former case $\sqrt{Z(k)}$ can be determined from $|\sqrt{Z(k)}|$ by looking at the graph of the latter near k_1. By continuing in this manner, we can obtain $\sqrt{Z(k)}$ from $|\sqrt{Z(k)}|$ in each of the remaining intervals $[k_m, k_{m+1}]$ for $m \geq 2$. Let $F_n(k)$ denote the quantity whose real part coincides with (3.14) and whose imaginary part is defined as

$$\text{Im}\,\{F_n(k)\} = \begin{cases} -\frac{1}{2}\sqrt{Z(k)}, & k \in [0, k_n], \\ -\frac{1}{2}|\sqrt{Z(k)}|, & k \in [k_n, +\infty), \end{cases} \tag{3.17}$$

where k_n is the n-th positive zero of Z. The set of k_n values is either finite or countably many. The quantity $F_n(k)$ becomes a better approximation to $F(k)$ as n increases. By using F_n instead of F, we can recover L_2 approximately. Then V_2 can be obtained approximately from the resulting L_2 by one of the numerical algorithms available. In Section 4 we illustrate the recovery of V_2 from F_n by using the algorithm of [Sa93].

In the absence of bound states, if V and V_1 are both generic, then V_2 must also be generic [AKV96]. With the help of (3.11), (3.16), and (2.5), we can summarize our findings as follows.

Theorem 3.3 Let $V \in L^1_1(\mathbf{R})$ be a generic potential, and let V_1 and V_2 be its fragments without bound states and contained on the left and right half-lines, respectively. If V_1 is also generic, then F defined in (2.5) is uniquely determined in terms of $\{|R_1|, |L_2|, |L|\}$ in such a way that $\text{Re}\,\{F(k)\}$ is given by (3.14) and $\text{Im}\,\{F(k)\}$ is given by

$$\text{Im}\,\{F(k)\} = -\frac{1}{2}\sqrt{Z(k)}, \tag{3.18}$$

where Z is the quantity given in (3.11). Moreover, the unique L_2 can be recovered from $\{R_1, |L_2|, |L|\}$ by using (3.14) and (3.18) in (2.10).

Next we illustrate the recovery of L_2 from $\{R_1, |L_2|, |L|\}$ by using the method presented in this section.

Example 3.4 Let us use the same scattering data as in (2.13) and (2.14). From (3.14) we get

$$\operatorname{Re}\{F(k)\} = \frac{k^2\,(16k^6 + 20k^4 + 32k^2 + 157)}{(4k^4 + 4k^2 + 9)(4k^4 + k^2 + 4)}, \tag{3.19}$$

and using (3.5) and (3.8) we obtain

$$Z(k) = \frac{144k^2(14k^2 - 17)^2}{(4k^4 + 4k^2 + 9)^2(4k^4 + k^2 + 4)^2}.$$

Hence $Z(k)$ has one positive zero and we have

$$\sqrt{Z(k)} = \frac{12k(17 - 14k^2)}{(4k^4 + 4k^2 + 9)(4k^4 + k^2 + 4)}, \tag{3.20}$$

using (3.18), (3.19), and (3.20), we get

$$F(k) = \frac{k(16k^7 + 20k^5 + 32k^3 + 157k + 84ik^2 - 102i)}{(4k^4 + 4k^2 + 9)(4k^4 + k^2 + 4)}. \tag{3.21}$$

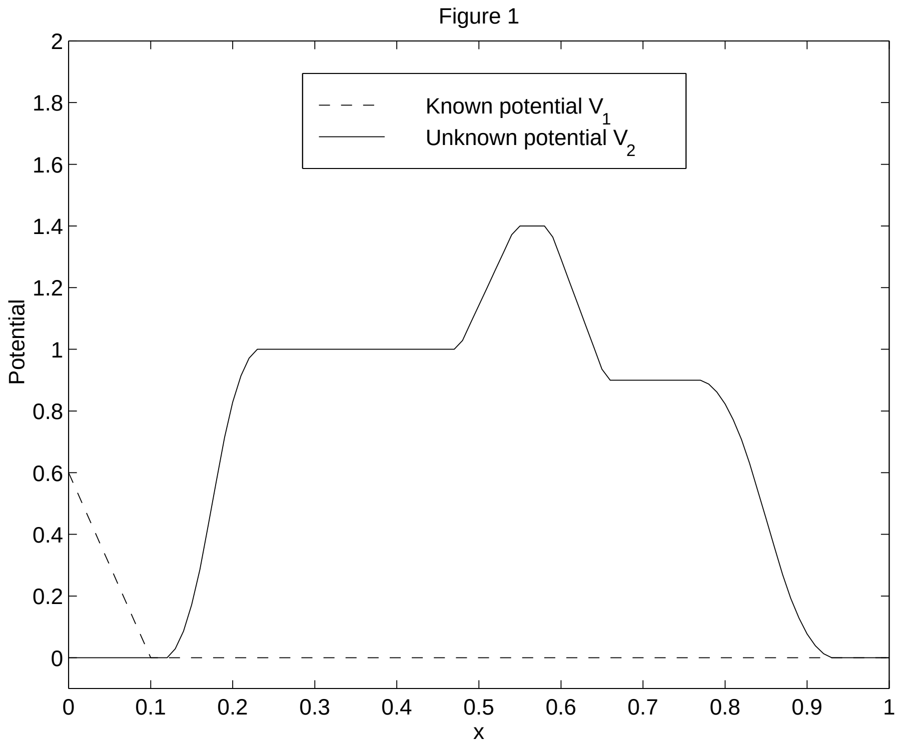
Using (2.14) and (3.21) in (2.10), after simplification, we get

$$L_2(k) = \frac{3}{2k^2 + 4ik - 3},$$

which agrees with (2.15) and corresponds to the potential in (2.16).

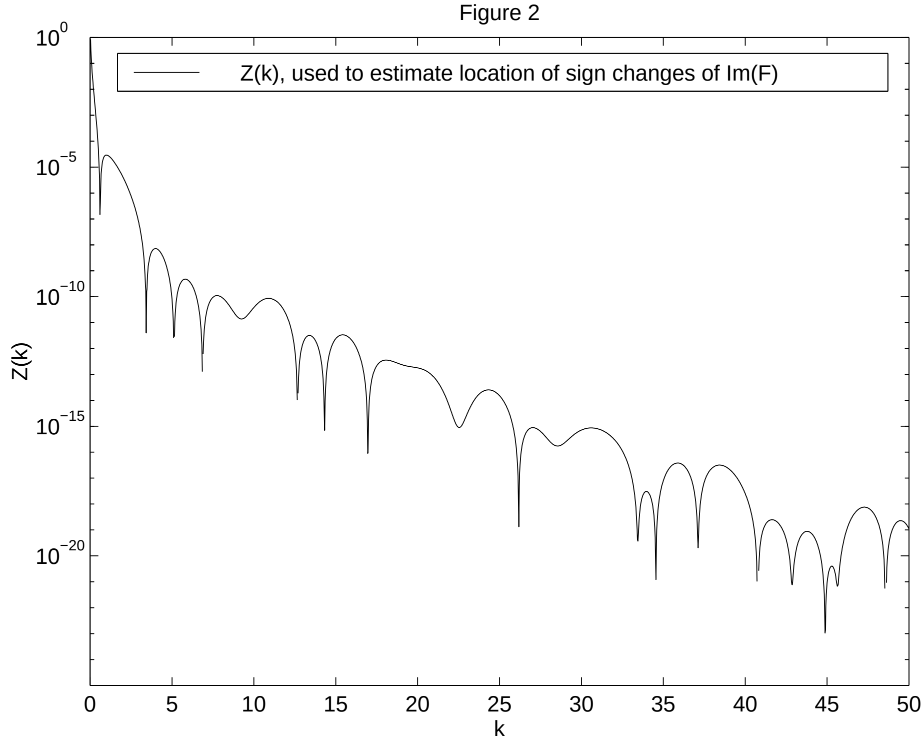
4. NUMERICAL EXAMPLE

In this section we give an example of numerical solution of the inverse scattering problem, based on the ideas of Section 3. The potential fragments V_1 and V_2 are displayed in Figure 1. The direct scattering data $\{R_1, |L_2|, |L|\}$ were generated at $k = .025j$ with $j = 1, \cdots, 2000$ using a method based on numerical solution of the Schrödinger equation (1.1).



From (2.4) and the given data we clearly know $|T|, |T_2|$, and $|T_1|$, thus we can immediately compute the functions Z in (3.11) and $\text{Re}\{F(k)\}$ in (3.14). Next we need to compute $\text{Im}\{F(k)\}$ in (3.17) which requires that we find $\{k_n\}$, the positive zeros of $Z(k)$. Due to the finite sampling rate, errors in data and in discretization, it is likely that no actual zeros will be found; so what is really meant here is that these locations must be estimated as best we can from the available values of $Z(k)$. The easiest way to do this is to examine a plot and/or listing of $\log Z(k)$ in which the approximate zeros of $Z(k)$ will appear as highly localized cusps, or relative minima. In Figure 2 we show the graph of $\log Z(k)$ for our example. This is the one step in the reconstruction procedure which is not completely automatic, and may indeed be difficult to carry out accurately if data are not very accurate or sparsely sampled. We remark however, that it is less crucial to correctly identify the zeros k_n at higher k values, as indicated below.

Figure 2



Once the above steps have been carried out, we then have an approximation for $F(k)$, and using (2.10) we get the full complex reflection coefficient L_2. We can now use one of the known methods of solving the standard inverse scattering problem to recover the potential V_2. Here we have used the method of [Sa93].

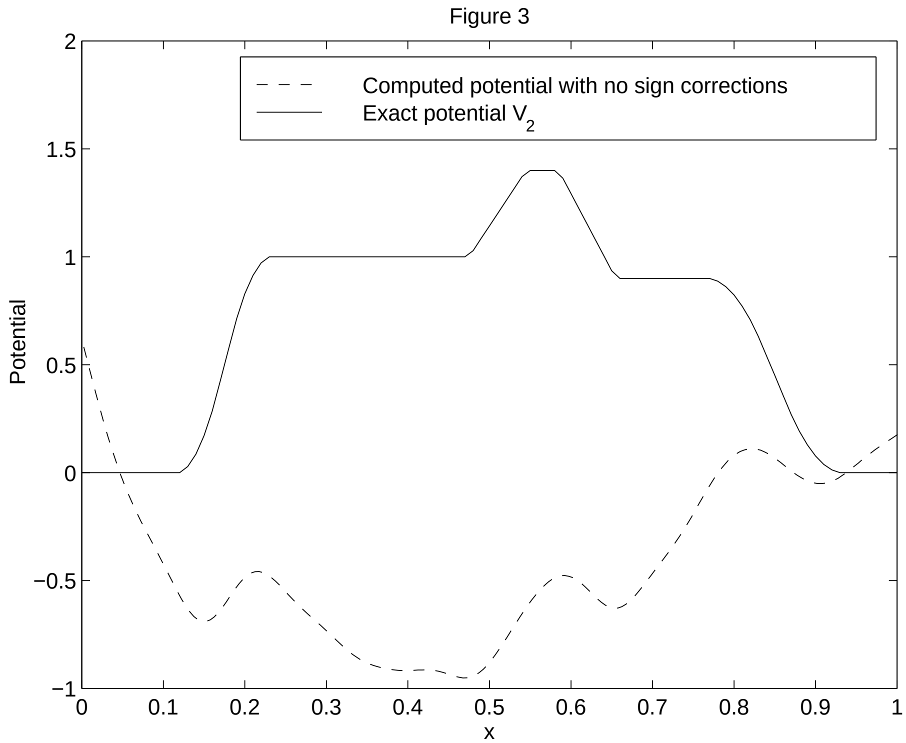


Figure 3 shows the (highly inaccurate) potential which we get if we do not take into account the sign changes of $\text{Im}\,\{F(k)\}$. By this we mean that $F(k)$ and subsequently $L_2(k)$ are computed using only $\text{Im}\,\{F(k)\} = -\frac{1}{2}\,|\sqrt{Z(k)}|$ for all k. In Figure 4 we show the potential obtained if we correct the sign of $\text{Im}\,\{F(k)\}$ only on the first interval (k_1, k_2) (i.e. $(0.6, 3.425)$ in this example) on which there is a sign change. Note that the approximation of V_2 is considerably improved by this one correction. Finally in Figure 5 we show the computed potential when the sign of $\text{Im}\,\{F(k)\}$ is chosen as described above for all k in the data set $0 < k < 50$.

Figure 4

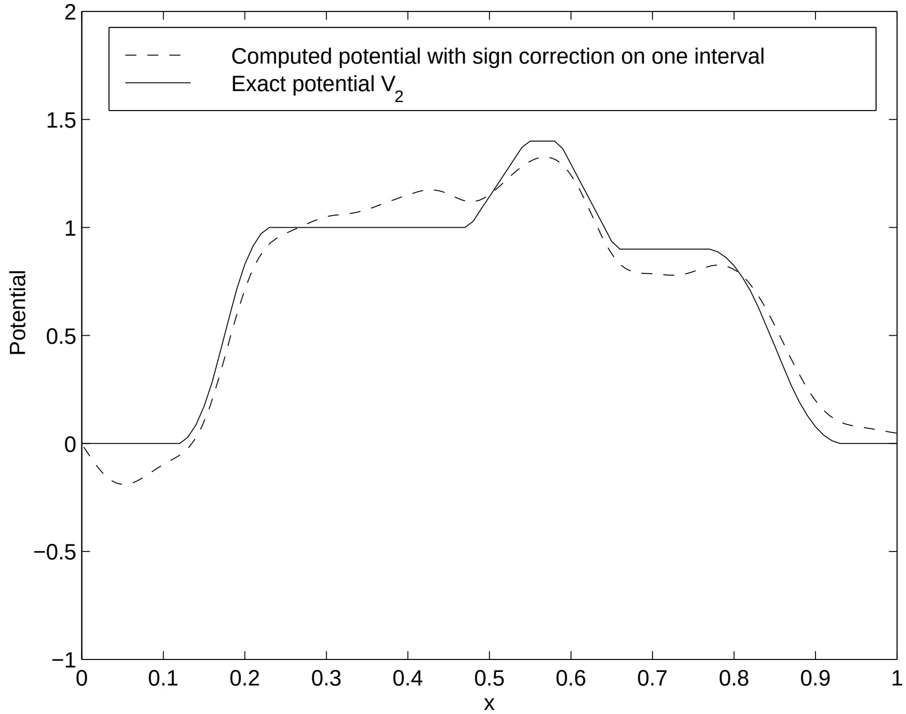
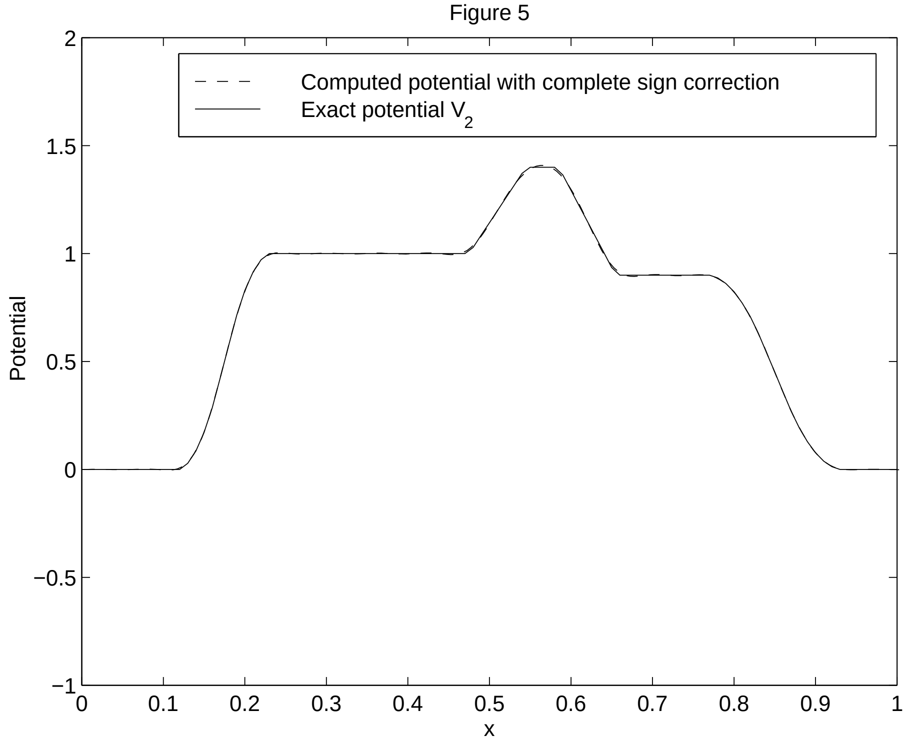


Figure 5



We remark finally that in principle it is possible to compute the function $F(k)$ directly from the Hilbert transform formula (2.9), and this may even seem preferable since it is completely unambiguous, requiring no determination of sign changes, as was needed in the method just discussed. Nevertheless the use of (2.9) will in general lead to a considerably less accurate reconstruction because of errors which arise in computing the Hilbert transform of the sampled function in the integrand of (2.9), which are then amplified by use of the formula (2.10) for L_2.

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