INVERSION OF REFLECTIVITY DATA FOR NONDECAYING POTENTIALS

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Abstract: The recovery of material properties of thin films is considered by probing them with neutron beams or X-rays. The interaction between the beam and the thin film is described by the one-dimensional Schrödinger equation with an optical potential that is supported in the right half-line and asymptotic to a positive constant. The reconstruction of such a potential is studied in terms of the scattering data consisting of the magnitude of the reflection coefficient from the left, a known potential placed to the left of the unknown potential, and the magnitude of the reflection coefficient for the combined potential. A previous method utilizing three sets of reflectivity measurements is generalized to potentials not decaying at infinity, and the precise conditions are indicated for the validity of this method. It is shown that two sets of reflectivity measurements, instead of three, are sufficient for the unique reconstruction. Some analytical and computational methods are provided for the recovery of the unknown potential and the phase of the corresponding reflection coefficient. The recovery is illustrated with some numerical examples.

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1. INTRODUCTION

The surface and interfacial properties of thin films can be described by an optical potential. Determining the optical potential is one of the most challenging tasks in materials science. A powerful tool developed to determine material properties is the use of reflectivity measurements obtained with neutron beams or X-rays (see e.g. [1-3] and the references therein), and such measurements have been utilized to study bonding of polymer components, polymer diffusion, magnetic films, high-temperature superconductors, diffusion of hydrogen in thin films, chemical modifications due to electrolytic charging, and other processes in materials science. When the beam strikes a material sample, it interacts with the nuclei and the magnetic moments at the surface of the sample and underneath, and the scattered beam contains information related to the atomic, chemical, and magnetic properties of the material. Using a device known as the reflectometer, the intensity of the reflected beam is measured in order to analyze the material properties.

The reflected beam is identified by a reflection coefficient, which is a complex-valued function of the energy of the beam, and the material properties are represented by the optical potential, which is a function of the distance from the surface. Under appropriate conditions (which are known to be satisfied in real experiments), knowledge of the reflection coefficient determines the optical potential. In reality one cannot measure the reflection coefficient but can only measure the reflectivity, the amplitude of the reflection coefficient, without its phase. The determination of a reflection coefficient from its amplitude is thus equivalent to obtaining the material properties using reflectivity measurements taken by reflectometers.

Mathematically, the interaction of the beam with the material is governed by 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 k^2 corresponds to the beam energy, the potential V is real valued and may be written as $V = V_1 + V_2$ with V_1 being supported in $\mathbf{R}^-$, V_2 supported in $\mathbf{R}^+$, and

$$V_1 \in L^1_1(\mathbf{R}^-), \qquad V_2 - c^2 \in L^1_1(\mathbf{R}^+), \tag{1.2}$$

for some nonnegative c. Our main interest is the case $c > 0$; we include the case $c = 0$ to emphasize that our results remain valid also when $c = 0$. In fact, most physical applications in materials science correspond to the case $c > 0$. In our notation, the prime denotes the derivative with respect to the spatial variable x, $\mathbf{R}^- = (-\infty, 0)$, $\mathbf{R}^+ = (0, +\infty)$, and $L^1_1(I)$ is the set of measurable functions f on an interval I such that $\int_I dx\,(1+|x|)\,|f(x)|$ is finite.

The scattering states of (1.1) correspond to its solutions behaving like $e^{\pm ikx}$ as $x \to -\infty$ and like $e^{\pm i\gamma x}$ as $x \to +\infty$, where

$$\gamma = \sqrt{k^2 - c^2}, \tag{1.3}$$

and it is understood that we use the branch of the square root function with $\operatorname{Im}\gamma \geq 0$. On the other hand, 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. Our primary aim in this paper is to present useful methods to recover material properties using probing beams, and in such applications bound states do not occur. Thus, throughout our paper we will assume that the potentials considered are free of bound states. For the treatment when bound states are involved, we refer the reader to [4], where further mathematical theory is developed.

The direct scattering problem for (1.1) is to determine the scattering coefficients (that are defined in terms of the spatial asymptotics of the scattering solutions as $x \to \pm\infty$) once the potential is known, whereas the inverse scattering problem is to recover the potential in terms of an appropriate set of scattering data related to the scattering coefficients. Such direct and inverse scattering problems for (1.1) were analyzed by Buslaev and Fomin [5], Legendre [6], and by Cohen and Kappeler [7]. The case $c = 0$ is the classical situation (see e.g. [8-11]) and the appropriate scattering data to recover V in (1.1) consist of a reflection coefficient. When $c > 0$, the appropriate scattering data are summarized in Theorem 2.2. We will refer to the cases $c = 0$ and $c > 0$ as the decaying and nondecaying cases, respectively, thinking that V vanishes in the L^1_1-sense as $x \to +\infty$ in the former case and that V approaches the positive value c in the L^1_1-sense as $x \to +\infty$ in the latter.

We are interested in a different formulation of the inverse scattering problem for (1.1), namely in the recovery of V_2 when the given data consist of V_1, the amplitude of a reflection coefficient for V_2, and the amplitude of the reflection coefficient for $V_1 + V_2$. We will refer to such scattering data as the two-measurement data, thinking that we measure the reflectivity for V_2 twice: once for V_2 alone and next in combination with some known potential V_1. In case the scattering data also contain a third measurement of the reflectivity for V_2 in combination with some other potential $\tilde{V}_1$ replacing V_1, we will call the resulting scattering data the three-measurement data. In applications in materials science, V_2 is the unknown potential or the scattering length density we seek to determine, and V_1 and $\tilde{V}_1$ are known layers we are able to place in front of V_2, i.e. between the radiation source and the unknown sample whose properties we seek to determine from the indicated data. There are several previous studies on this problem when $c = 0$, see [12-16]. Thus the main contribution of this paper is to analyze the situation when $c > 0$. As we will see, the most important difference is that for $k \in [0, c)$ the extra measurements provide no additional information about the phase of the reflection coefficient. Since this set of phase data is eventually needed for the recovery of V_2, it must be inferred in some other way.

This paper is organized as follows. In Section 2 we summarize the relevant facts related to the scattering coefficients corresponding to V and the recovery of V. In Section 3 we consider the recovery of V_2 from the three-measurement data, and in Section 4 we indicate the unique determination of V_2 from the two-measurement data. Finally, in Section 5 we discuss some numerical procedures to recover V_2 from both two and three sets of reflectivity measurements and illustrate the recovery by some numerical examples.

2. PRELIMINARIES

In this section we establish notation, give precise definitions, and recall properties of the scattering data which we will need. Much of this material may be found in [5-7] and in some other cases it is a simple adaptation of arguments in [8-11].

The Jost solution from the left, $f_l(k,x)$, associated with V is the solution of (1.1) satisfying

$$e^{-i\gamma x} f_l(k,x) = 1 + o(1), \quad e^{-i\gamma x} f_l'(k,x) = i\gamma + o(1), \qquad x \to +\infty,$$

where γ is the quantity defined in (1.3). The transmission and reflection coefficients from the left, T_l and L, can be defined in terms of the spatial asymptotics of $f_l(k,x)$ as

$$e^{-ikx}\, f_l(k,x) = \frac{1}{T_l(k)} + \frac{L(k)}{T_l(k)} e^{-2ikx} + o(1), \qquad x \to -\infty.$$

Similarly, transmission and reflection coefficients from the left, T_r and R, can be defined in terms of $f_r(k,x)$, the Jost solution from the right, as

$$e^{ikx}\, f_r(k,x) = 1 + o(1), \quad e^{ikx}\, f_r'(k,x) = -ik + o(1), \qquad x \to -\infty,$$

$$e^{i\gamma x}\, f_r(k,x) = \frac{1}{T_r(k)} + \frac{R(k)}{T_r(k)} e^{2i\gamma x}, \qquad x \to +\infty.$$

Equivalently, it is also possible to define the transmission and reflection coefficients in terms of Wronskian relations of $f_l(k,x)$ and $f_r(k,x)$ [5,7]. If $c \neq 0$, then T_r and T_l are not the same. We will have no need for T_r in what follows, so for simplicity of notation we will denote T_l by T. We then use obvious notation for the scattering data for V_1, $\tilde{V}_1$, and V_2; i.e. L_1, R_1, T_1 for V_1; $\tilde{L}_1$, $\tilde{R}_1$, $\tilde{T}_1$ for $\tilde{V}_1$; and L_2, R_2, T_2 for V_2.

Regardless of whether $c = 0$ or $c > 0$, there are two possible behaviors of $T(k)$ at $k = 0$; if $T(0) \neq 0$ the exceptional case occurs, and if $T(0) = 0$ the generic case occurs. In the rest of this paper we will consider only generic potentials because this condition is met in applications involving recovery of material properties using neutron beams or X-rays. We refer the reader to [4] for the treatment when exceptional potentials are involved.

For the decaying case, in an earlier paper [16] it was shown that L_2 for $k \in \mathbf{R}$ (and hence V_2) is recovered uniquely in terms of $\{R_1, |L_2|, |L|\}$ for $k \in [0, +\infty)$. Other related works [12-15] have discussed the recovery of the phase of L_2 using three measurements, i.e. $\{R_1, \tilde{R}_1, |L_2|, |L|, |\tilde{L}|\}$. All of these other methods are essentially local in k, that is to say the phase of L_2 at a given k value is determined from the indicated data at the same k value.

In the nondecaying case, we have $|L_2| \equiv 1$ and $|L| \equiv 1$ for $k \in [0, c]$ no matter what V_1 is, hence, except for revealing the value of c, the scattering data for small k cannot contain any information about V_2, and in particular we cannot expect to directly recover the phase of L_2 for $k \in (0, c)$ from the indicated data. As a theoretical matter we can overcome this obstacle by an analytic continuation argument, but some other kind of approach is needed for computational purposes.

We now summarize some of the known results [5,7] about the direct and inverse scattering problem for nondecaying potentials.

Theorem 2.1 (Direct problem) Let V_1, V_2, and V be generic potentials without bound states, where $V = V_1 + V_2$ and (1.2) holds for a given $c \geq 0$. Then, the quantities T, $k/T(k)$, R_1, and L_2 are analytic in the upper half complex plane $\mathbf{C}^+$ and are continuous in its closure $\overline{\mathbf{C}^+}$, and we have

$$T(-k) = T(k)^*, \quad L(-k) = L(k)^*, \qquad k \in \mathbf{R}, \tag{2.1}$$

$$L(k) = \frac{T(k)}{T(k)^*}, \qquad k \in [-c, c], \tag{2.2}$$

$$1 - |L(k)|^2 = \frac{\gamma}{k}|T(k)|^2, \qquad k \in \mathbf{R} \setminus (-c, c), \tag{2.3}$$

$$R(k) = -\frac{T(k)\,L(k)^*}{T(k)^*}, \qquad k \in \mathbf{R}, \tag{2.4}$$

where the asterisk denotes complex conjugation. Both R and L are continuous for $k \in \mathbf{R}$, they vanish as $o(1/k)$ when $k \to \pm\infty$, and we have $R(0) = L(0) = -1$. Moreover, $T(k)$ is nonzero for $k \in \mathbf{R} \setminus \{0\}$, $T(k) = 1 + O(1/k)$ as $k \to \infty$ in $\overline{\mathbf{C}^+}$, and $T(k)$ vanishes linearly as $k \to 0$ in $\overline{\mathbf{C}^+}$.

Theorem 2.2 (Inverse problem) Let V_1, V_2, and V be generic potentials without bound states, where $V = V_1 + V_2$ and (1.2) holds for a given $c \geq 0$. Then V is uniquely determined by either

(i) $L(k)$ for $k \in (0, +\infty)$,

or

(ii) c, $R(k)$ for $k \in (c, +\infty)$, and $|T(k)|$ for $k \in (0, c)$.

We note that the value of c can be obtained from $|L_2|$ (or equivalently from $|L|$) as

$$c = \sup\{a \in \mathbf{R}^+ : \ |L_2(k)| = 1, \quad k \in [0, a)\}.$$

Let us also remark that [17] is specifically concerned with numerical computation of V_2 given L_2 for $k \in (0, +\infty)$.

3. THREE MEASUREMENTS

In this section we consider the determination of the potential V_2 in terms of the three-measurement data. When $c = 0$ such a result has been derived in some earlier works [12,14], formally at least, based on the recovery of $L_2(k)$ at any fixed real value of k by using the intersection of three circles on the complex plane. In Corollary 3.2 we describe the exact conditions for the three-circle method to be valid or to fail. In Example 3.3 we present two potentials for which the three-circle method will not work at any k value. The extension to $c > 0$ is relatively straightforward, but we are not aware of any precise statements along these lines in earlier works.

Define the transition matrix Λ for $k \in \mathbf{R} \setminus \{0\}$ corresponding to V and the transition matrices Λ_j corresponding to V_j for $j = 1, 2$ as

$$\Lambda(k) = \begin{bmatrix} \dfrac{1}{T(k)} & \dfrac{L(k)^*}{T(k)^*} \\ \dfrac{L(k)}{T(k)} & \dfrac{1}{T(k)^*} \end{bmatrix}, \qquad \Lambda_j(k) = \begin{bmatrix} \dfrac{1}{T_j(k)} & \dfrac{L_j(k)^*}{T_j(k)^*} \\ \dfrac{L_j(k)}{T_j(k)} & \dfrac{1}{T_j(k)^*} \end{bmatrix}.$$

It is possible to express Λ and Λ_j in terms of the reflection coefficients R and R_j from the right by using (2.4) and

$$R_j(k) = -\frac{L_j(k)^* \, T_j(k)}{T_j(k)^*}, \qquad k \in \mathbf{R}.$$

We have

$$\Lambda(k) = \Lambda_1(k)\, \Lambda_2(k), \qquad k \in \mathbf{R} \setminus \{0\}. \tag{3.1}$$

The proof of (3.1) can be obtained in a similar way as in the case $c = 0$ (see e.g. [18]) and will not be given here. Note that (2.2) implies that the columns of Λ become identical when $k \in [-c, c] \setminus \{0\}$, and the same is true for the columns of Λ_2. Note also that (3.1) is equivalent to

$$\frac{1}{T(k)} = \frac{1 - R_1(k)\, L_2(k)}{T_1(k)\, T_2(k)}, \qquad k \in \mathbf{R} \setminus \{0\}, \tag{3.2}$$

$$\frac{L(k)}{T(k)} = \frac{L_2(k) - R_1(k)^*}{T_1(k)^* \, T_2(k)}, \qquad k \in \mathbf{R} \setminus \{0\}. \tag{3.3}$$

It is known [13] that a measurement of reflectivity $|L(k)|$, when a known layer is placed in front of the unknown sample, serves to locate the reflection coefficient $L_2(k)$ on a certain circle in the complex plane. There is actually a family of such circles:

Proposition 3.1 Assume V_1 and V_2 satisfy (1.2), and fix $t \in \mathbf{R}$ and $k \in \mathbf{R} \setminus [-c, c]$. Then $L_2(k)$ is located on the circle in the complex plane with center $t\, R_1(k)^*$ and radius $\rho = \rho(t, R_1(k))$, where

$$\rho^2 = t \frac{|L|^2 \,(1 - |R_1|^2)\,(1 - |L_2|^2)}{1 - |L|^2} + (t^2 - t)\, |R_1|^2 + (1 - t)\, |L_2|^2. \tag{3.4}$$

PROOF: From (2.3) and (3.3) we get

$$|L_2 - R_1^*|^2 = \frac{|L|^2\,(1-|R_1|^2)\,(1-|L_2|^2)}{1-|L|^2}, \qquad k \in \mathbf{R}\setminus[-c,c]. \tag{3.5}$$

We have

$$|L_2 - R_1^*|^2 = |L_2|^2 + |R_1^*|^2 - 2\,\mathrm{Re}\,\{L_2 R_1^*\}, \tag{3.6}$$

$$|L_2 - tR_1^*|^2 = |L_2|^2 + t^2\,|R_1^*|^2 - 2t\,\mathrm{Re}\,\{L_2 R_1^*\}, \tag{3.7}$$

Multiplying (3.6) by $-t$ and adding the result to (3.7) we get

$$|L_2 - tR_1^*|^2 = t\,|L_2 - R_1^*|^2 + (t^2-t)\,|R_1^*|^2 + (1-t)\,|L_2|^2. \tag{3.8}$$

Thus, from (3.5) and (3.8), we obtain $|L_2 - t\,R_1^*| = \rho$ and hence (3.4). ∎

We remark that the choice

$$t = \frac{1-|L|^2}{1-|L|^2|L_1|^2}$$

gives the circle used in [12,13]. From Proposition 3.1 we see that any two of the one-parameter circles, where t is the parameter, intersect at $L_2(k)$ and at its image with respect to the line through the origin and $R_1(k)^*$. Let $t,\tilde t \in \mathbf{R}$ and let R_1 and $\tilde R_1$ be two reflection coefficients such that 0, $R_1(k)$, and $\tilde R_1(k)$ are not located on the same line, i.e. $R_1(k)\,\tilde R_1(k)^*$ is not real. For each fixed $k\in\mathbf{R}\setminus[-c,c]$, we can obtain $L_2(k)$ uniquely as the intersection of the circle centered at 0 with radius $|L_2(k)|$, the circle centered at $t\,R_1(k)^*$ with radius $\rho(t,R_1(k))$, and the circle centered at $\tilde t\,\tilde R_1(k)^*$ with radius $\rho(\tilde t,\tilde R_1(k))$. Thus, we have

$$L_2 = \frac{R_1 - \tilde R_1 + |L_2|^2\,R_1\,\tilde R_1\,[\tilde R_1^* - R_1^*] + [1-|L_2|^2]\,G}{2i\,\mathrm{Im}\,\{R_1\,\tilde R_1^*\}}, \qquad k\in\mathbf{R}\setminus[-c,c], \tag{3.9}$$

where we have defined

$$G = \frac{\tilde R_1\,(1-|R_1|^2)}{1-|L|^2} - \frac{R_1\,(1-|\tilde R_1|^2)}{1-|\tilde L|^2}.$$

Note that G is well defined because, as seen from (2.3), both $|L|$ and $|\tilde{L}|$ are strictly less than 1 for $k \in \mathbf{R} \setminus [-c, c]$. ∎

From (3.9) we obtain the following result.

Corollary 3.2 Assume that V_1 and $\tilde{V}_1$ belong to $L_1^1(\mathbf{R}^-)$ and that V_2 satisfies (1.2). Then, $L_2(k)$ is uniquely determined at any value of k for $k \in \mathbf{R} \setminus (-c, c)$ by

$$\{R_1(k), \tilde{R}_1(k), |L_2(k)|, |L(k)|, |\tilde{L}(k)|\}, \qquad k \in (c, +\infty), \tag{3.10}$$

if and only if $\mathrm{Im}\,\{R_1\,\tilde{R}_1^*\}$ is nonzero at that k value.

In the next example, we elaborate on the condition $\mathrm{Im}\,\{R_1\,\tilde{R}_1^*\} = 0$. Note that this condition is equivalent to saying that $R_1(k)$ and $\tilde{R}_1(k)$ either have the same argument or their arguments differ by π. We show that it is possible to have two distinct potentials V_1 and $\tilde{V}_1$ for which $\arg\{R_1(k)\} = \arg\{\tilde{R}_1(k)\}$ for all $k \in \mathbf{R}$.

Example 3.3 Let

$$R_1(k) = \frac{(k-2i)^2}{2(k+i)^2(k+2i)(2k+i)}, \qquad \tilde{R}_1(k) = \frac{8(k-i)^2}{(k+2i)^3(2k+i)}. \tag{3.10}$$

Note that $R_1(0) = \tilde{R}_1(0) = -1$, both $|R_1(k)|$ and $|\tilde{R}_1(k)|$ are strictly less than one for $k \in \mathbf{R} \setminus \{0\}$, both R_1 and $\tilde{R}_1$ are analytic in $\mathbf{C}^+$, and they both are $O(1/k^2)$ as $k \to \infty$ in $\overline{\mathbf{C}^+}$. We have

$$R_1(k)\,\tilde{R}_1(k)^* = \frac{4}{(k^2+4)(4k^2+1)}, \qquad k \in \mathbf{R},$$

or equivalently

$$\tilde{R}_1(k) = \frac{16(k^2+1)^2}{(k^2+4)^2}\,R_1(k), \qquad k \in \mathbf{R}.$$

The corresponding potentials V_1 and $\tilde{V}_1$ are generic, do not support any bound states, vanish for $x > 0$, and exponentially decay as $x \to -\infty$. Since R_1 and $\tilde{R}_1$ are rational functions of k, the so-called Bargmann potentials V_1 and $\tilde{V}_1$ can be constructed explicitly, although such constructions are tedious and the resulting expressions are complicated.

Proposition 3.4 Assume that V_1 and $\tilde{V}_1$ are nontrivial potentials belonging to $L_1^1(\mathbf{R}^-)$ and that V_2 is a potential without bound states satisfying (1.2). If $\mathrm{Im}\,\{R_1\tilde{R}_1^*\}$ is nonzero for almost all k values in some interval in $(c,+\infty)$, then V_2 is uniquely determined by the scattering data consisting of c and (3.10). In particular, the same scattering data uniquely determine L_2 for $k\in\overline{\mathbf{C}^+}$.

PROOF: By Corollary 3.2 the values of $L_2(k)$ are uniquely determined in some interval in $(c,+\infty)$, and L_2 is analytic in $\mathbf{C}^+$ and continuous in $\overline{\mathbf{C}^+}$ as indicated in Theorem 2.1. Hence by analytic continuation, L_2 is uniquely determined in all of $\overline{\mathbf{C}^+}$ by its values in some interval on the real axis. By Theorem 2.2, it then follows that V_2 is uniquely determined. ∎

In Corollary 3.2 we have seen the limitation of the three-circle method; if $\mathrm{Im}\,\{R_1\tilde{R}_1^*\}$ vanishes at some k value, then the three-measurement data in (3.10) at that k value reduce to the two-measurement data that will be analyzed in Section 4, where we show that one can get along without the third measurement and that the two-measurement data uniquely determine L_2 for all $k\in\mathbf{R}$ and hence V_2. Thus, even though the three-circle method may fail at some or all k values in $(c,+\infty)$, the restriction $\mathrm{Im}\,\{R_1(k)\,\tilde{R}_1(k)^*\}\neq 0$ in Proposition 3.4 can be omitted, and hence the three-measurement data in (3.10) uniquely determine V_2.

4. TWO MEASUREMENTS

In Section 3 we have studied the recovery of L_2 and hence V_2 in terms of three-measurement scattering data. In this section we show that actually two measurements suffice; more precisely, we can uniquely determine L_2 for $k\in\mathbf{R}$, and subsequently V_2, by the two-measurement data $\{R_1,|L_2|,|L|\}$ for $k\in[0,+\infty)$. Thus one measurement, $|L_2|$, corresponds to the initial layer $V_1\equiv 0$, and the other measurement corresponds to some other choice of V_1, which we assume is not identically zero.

It is more convenient to transform the centers of the one-parameter family of circles used in deriving (3.9) from their location on the complex plane to the real axis. For this we proceed as follows. Let us define

$$F(k) = 1 - R_1(k)\, L_2(k), \qquad k \in \mathbf{R}. \tag{4.1}$$

Clearly, when R_1 (or equivalently V_1) is known, knowledge of L_2 is equivalent to knowledge of F. From (3.2) we see that $F = T_1 T_2 / T$, and hence in the absence of bound states F can be extended analytically from $\mathbf{R}$ to $\mathbf{C}^+$. The construction of F is much easier than a direct construction of L_2 because the analytical extension of F has no zeros in $\mathbf{C}^+$, whereas this is in general not true for L_2.

Using Proposition 3.1 we obtain the following result.

Corollary 4.1 Assume V_1 and V_2 satisfy (1.2), and fix $s \in \mathbf{R}$ and $k \in \mathbf{R} \backslash [-c, c]$. Then $F(k)$ is located on the circle in the complex plane with center $s + i0$ and radius $\varrho = \varrho(s, R_1(k))$, where

$$\varrho^2 = s^2 + |R_1|^2\, |L_2|^2 - s \left[|R_1|^2 + |L_2|^2 + \frac{|L|^2\,(1 - |R_1|^2)\,(1 - |L_2|^2)}{1 - |L|^2} \right].$$

Any two circles from the one-parameter family with s being the parameter intersect at $F(k)$ and $F(k)^*$.

Theorem 4.2 Assume that V_1 and V_2 are free of bound states and satisfy (1.2) and that $V_1 \not\equiv 0$. Then V_2 is uniquely determined by the scattering data consisting of c and $\{R_1, |L|, |L_2|\}$ for $k \in (c, +\infty)$. Moreover, the same scattering data uniquely determine F and L_2 for $k \in \overline{\mathbf{C}^+}$.

PROOF: Because of (4.1) and analytic continuation, it is sufficient to prove that F is uniquely determined for $k \in (c, +\infty)$. From Corollary 4.1, by using any two different values of the parameter s, it follows that $F(k)$ at any fixed $k \in (c, +\infty)$ is uniquely determined by the two-measurement scattering data at that k value, up to the sign in $\mathrm{Im}\,\{F(k)\}$. From Theorem 2.1 we see that $F - 1$ is analytic in $\mathbf{C}^+$ and continuous in $\overline{\mathbf{C}^+}$, and furthermore $|F(k) - 1| = O(1/k^2)$ as $k \to \infty$ in $\overline{\mathbf{C}^+}$.

Now suppose that there exist two distinct potentials V_2 and $\tilde{V}_2$ both corresponding to the same scattering data. Define F as in (4.1), and let $\tilde{F} = 1 - R_1\tilde{L}_2$, where $\tilde{L}_2$ is the reflection coefficient from the left for $\tilde{V}_2$. We cannot have $F = \tilde{F}$ on any interval in $\mathbf{R}$, since otherwise by analytic continuation we would have $F = \tilde{F}$ on all of $\mathbf{R}$, which would imply $V_2 = \tilde{V}_2$. On the other hand, by the above discussion F is uniquely determined up to the sign of its imaginary part for $k > c$, hence we must have $\tilde{F}(k) = F^*(k)$ for $k > c$. Since F^* has an analytic extension to the lower half plane, it follows that $\tilde{F}$ has an extension which is continuous in the entire complex plane, and analytic in the upper and lower half planes, hence entire. Since we also then have $|\tilde{F}(k) - 1| = O(1/k^2)$ as $k \to \infty$ in $\mathbf{C}$, it follows that $\tilde{F}$ is a bounded entire function, hence constant, a contradiction. ▮

As a computational matter, it is clear that the determination of the correct sign of $\mathrm{Im}\,\{F(k)\}$ is the main difficulty. Such a procedure was studied in [16] for the case $c = 0$, and for the most part can be adapted to the case $c > 0$. We will only give an outline and refer the reader to [16] for details.

Given the two-measurement scattering data $\{R_1, |L_2|, |L|\}$ for $k \in [0, +\infty)$, we first evaluate $A(k)$ defined by

$$(4.2)\quad A(k) = \frac{1}{2}\left[1 + |R_1(k)|^2\,|L_2(k)|^2 - \frac{[1 - |R_1(k)|^2][1 - |L_2(k)|^2]}{1 - |L(k)|^2}\right], \qquad k \in (c, +\infty).$$

The real part of $F(k)$ is then given by

$$(4.3)\qquad \mathrm{Re}\,\{F(k)\} = 1 - A(k), \qquad k \in (c, +\infty).$$

Next we construct $Z(k)$ defined as

$$(4.4)\qquad Z(k) = 4\,|R_1(k)|^2\,|L_2(k)|^2 - 4A(k)^2, \qquad k \in (c, +\infty).$$

The quantity Z in (4.4) is a nonnegative function of k on $(c, +\infty)$ and

$$[\mathrm{Im}\,\{F(k)\}]^2 = \frac{1}{4}\,Z(k), \qquad k \in (c, +\infty).$$

Thus we may compute $Z(k)$ explicitly from the given scattering data, and then examine its behavior in neighborhoods of its zeros to determine if a sign change of $\mathrm{Im}\, F$ is taking place. In principle, higher order zeros can clearly occur, in which case it may be quite difficult to decide if the order is even or odd (i.e. whether a sign change of $\mathrm{Im}\,\{F(k)\}$ actually occurs), but in practice all such zeros are simple, and so we may assume a sign change at any zero of Z. Of course, numerically exact zeros of Z do not occur either, so the real decision concerns which 'approximate zeros' of Z correspond to genuine zeros. See Section 4 of [16] for further discussion.

The above procedure for determining sign changes of $\mathrm{Im}\,\{F(k)\}$ still leaves us with the two candidates $F(k)$ and $F^*(k)$, either of which is uniquely determined by its value at a single point for which $Z(k) \neq 0$. In the case $c = 0$ the asymptotics of F as $k \to 0$ may be worked out in such a way as to determine the sign of $\mathrm{Im}\,\{F(k)\}$ in an interval $(0, k_0)$ and hence for all $k \in (0, +\infty)$. That is, of the two candidates for $F(k)$, one and only one has the proper behavior as $k \to 0$, namely $\arg\{F(0^+)\} = -\pi/2$. In the case $c > 0$ this is still true, but we do not have access to F or F^* for $k \in (0, c)$ except by analytic continuation, which is of no use numerically.

Nevertheless, as will be discussed in the next section, in order to eventually reconstruct the potential V_2, some method (at least implicitly) must be used for approximating L_2, and hence F for $k \in (0, c)$. Given the two candidates for F on $(c, +\infty)$, we can construct, via one of several possible methods of Section 5, two candidates on $(0, +\infty)$, and we may then check, for example, which of the two has the correct behavior as $k \to 0$. An alternative which may be useful is to observe that exactly one of the two candidates for $F - 1$ (equivalently for L_2) possesses the correct analyticity and decay properties in $\overline{\mathbf{C}^+}$ so that the Kramers-Kronig relations hold, i.e.

$$\mathrm{Re}\,\{F(k) - 1\} = \frac{1}{\pi}\,\mathrm{CPV}\int_{-\infty}^{\infty} dt\,\frac{\mathrm{Im}\,\{F(t)\}}{t-k},$$

$$\operatorname{Im}\{F(k)\} = -\frac{1}{\pi}\,\mathrm{CPV}\int_{-\infty}^{\infty} dt\,\frac{\operatorname{Re}\{F(t)-1\}}{t-k},$$

where CPV denotes the Cauchy principal value. In other words, the real and imaginary parts of $F-1$ (or of L_2) form a Hilbert-transform pair.

If we let

$$g(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, L_2(k)\, e^{-ikt}, \tag{4.5}$$

then the Hilbert-transform relation for L_2 is equivalent to the statement that $g(t) \equiv 0$ for $t < 0$ (this also follows directly from the Paley-Wiener theory). Since g is always computed as a part of our numerical solution technique, this is straightforward to check.

Another version of the two-measurement problem has been studied recently in [19], namely the case when V_1 is the unknown potential and reflectivity data are available for two different constant choices of V_2. The following was actually proved: If V_1 has compact support in the interval $(0, l)$ and if V_2 is taken to be a constant c^2 for two different choices of c, then the two reflectivity measurements uniquely determine $\operatorname{Re}\{R_1(k)\, e^{-2ikl}\}$ for k larger than the maximum of the two c values. The authors then argue, and support with the evidence of a numerical example, that V_1 can then be typically extracted. A proof that this is so can be given along the lines of Theorem 4.2. A special case is:

Theorem 4.3 Assume that V_1 has support in $\mathbf{R}^-$ and belongs to $L_1^1(\mathbf{R}^-)$; let $V_2(x) = c^2\, H(x)$, where $c > 0$ and $H(x)$ is the Heaviside function. Then V_1 is uniquely determined by the scattering data consisting of $\{|R_1|, |L|\}$ for $k \in (c, +\infty)$ and the value of c.

PROOF: First, note that we can use $|L_1|$ in our data instead of $|R_1|$ because $|L_1| = |R_1|$. By explicit computation we obtain

$$L_2(k) = \frac{k - \sqrt{k^2 - c^2}}{k + \sqrt{k^2 - c^2}}, \qquad k \in \mathbf{R}, \tag{4.6}$$

and hence from (4.1) we get

$$\operatorname{Re}\{F(k)\} = 1 - \frac{k - \sqrt{k^2 - c^2}}{k + \sqrt{k^2 - c^2}}\operatorname{Re}\{R_1(k)\}, \qquad k \in \mathbf{R} \setminus (-c, c). \tag{4.7}$$

Thus, from (4.2), (4.3), and (4.7), it follows that $\operatorname{Re}\{R_1(k)\}$ is uniquely determined by our data for $k \in (c, +\infty)$. Since $|R_1|$ is known, $\operatorname{Im}\{R_1(k)\}$ is determined up to a choice of sign. We can now show that R_1 is uniquely determined for all $k > 0$, and the argument is precisely the same as that in the proof of Theorem 4.2 with $F(k)$ replaced by $R_1(k)$. Finally, by classical inverse scattering theory, V_1 may be found from R_1. ∎

In the above proof the constancy of the back layer is used in only one essential way, namely that L_2 is real for $k > c$. Theorem 4.3 will thus remain valid for any other V_2 having the same property, or more generally it is valid providing only that L_2 is real (or imaginary) on some nontrivial interval (k_1, k_2). This theorem also remains valid if $e^{2ikb}L_2(k)$ is real (or imaginary) on some interval (k_1, k_2) and the support of V_1 is contained in $(-\infty, b)$ for some constant b; this is due to the fact that when a potential is shifted as $V(x) \mapsto V(x-b)$, the corresponding reflection coefficient changes as $L(k) \mapsto e^{2ikb}\, L(k)$.

Let $V_2(x) = c^2 H(x)$ and $\tilde{V}_2 = \tilde{c}^2 H(x)$ for $c \neq \tilde{c}$. Let the reflection coefficients L and $\tilde{L}$ correspond to V and $\tilde{V}$, respectively, where $V = V_1 + V_2$ and $\tilde{V} = V_1 + \tilde{V}_2$. Then, the proof of Theorem 4.3 can be modified to conclude that V_1 is uniquely determined by the values of c and $\tilde{c}$ and $\{|L|, |\tilde{L}|\}$ for $k > \max\{c, \tilde{c}\}$.

In fact, by switching the roles of R_1 and L_2 in the proof of Theorem 4.2, we obtain the following generalization of the result of Theorem 4.3, where V_2 need not be constant.

Corollary 4.4 Assume that V_1 and V_2 are generic potentials without bound states satisfying (1.2) for some $c \geq 0$. If $V_2 \not\equiv 0$, then V_1 is uniquely determined by the scattering data consisting of $\{|R_1|, L_2, |L|\}$ for $k \in (c, +\infty)$ and the value of c.

5. COMPUTATIONAL METHODS

In this section we discuss some aspects of numerical computation of V_2 using both two and three sets of reflectivity measurements. The reconstruction procedure when three measurements are available is clearly simpler, so we begin with this case. Recall that the potentials considered here are assumed free of bound states and generic.

We first note that even though Proposition 3.4 assures the uniqueness of V_2 if the condition $\mathrm{Im}\{R_1\tilde{R}_1^*\} \neq 0$ is satisfied for almost all k in some interval in $(c, +\infty)$, it is clear that the procedure may be very unstable if $\mathrm{Im}\{R_1\tilde{R}_1^*\}$ is close to zero for $k > c$, i.e. if 0, $R_1(k)$, and $\tilde{R}_1(k)$ are nearly collinear on the complex plane for $k > c$. To see when this might happen, let $\hat{V}(k) = \int_{-\infty}^{\infty} dx\, V(x)\, e^{-ikx}$ denote the Fourier transform of a potential $V \in L_1^1(\mathbf{R})$. Then, from the Born approximation it follows that $\hat{V}(k) \approx ikR(k/2)$ for large k or weak potentials, where R is the reflection coefficient from the right for V. Thus if V_1 and $\tilde{V}_1$ are linearly dependent on $\mathbf{R}$, we will have 0, $R_1(k)$, and $\tilde{R}_1(k)$ nearly collinear, for all frequencies in the case of weak scattering, or at high frequencies in any case. Thus, we should avoid such choices of V_1 and $\tilde{V}_1$, e.g. we should not choose V_1 and $\tilde{V}_1$ to be two different positive constants with the same support interval, even though the uniqueness result of Proposition 3.4 certainly applies in this case. On the other hand, choosing V_1 and $\tilde{V}_1$ to be the same constant with different support intervals should produce good numerical inversion results. This kind of instability will not arise in connection with the two measurement method of Section 4, but the numerical implementation of that method is somewhat more complicated in other respects.

Given a set of three measurements at some fixed value of $k \in (c, +\infty)$, leading to three circles Γ_1, Γ_2, and Γ_3 in the complex plane on which $L_2(k)$ must lie, our first task in the inversion process is to locate the point of intersection of these three circles. In practice, due to data error, there may not actually be any point of intersection, and we must nevertheless select a method to approximate the true value of $L_2(k)$. One straightforward approach is simply to minimize a suitable cost functional, such as

$$C(z) = \sum_{j=1}^{3} (|z - \gamma_j|^2 - \rho_j^2)^2$$

as a nonlinear least-square problem, where γ_j denotes the center and ρ_j the radius of Γ_j.

A better approach is to compute first the lines in the complex plane connecting the two points of intersection of each pair of circles. In this way we get three linear equations for the two unknowns, i.e. the real and imaginary parts of $L_2(k)$, and the system can then be solved as a linear least-square problem. Of course one could also select any two of the three equations, and solve the corresponding system of two equations, but treating the three equations in a symmetric manner seems preferable and entails little additional computational cost. Using $|L_2(k) - \gamma_j|^2 = \rho_j^2$ with $j = 1, 2, 3$ and subtracting the equations for j and l, we get the linear equations

$$[\mathrm{Re}\,\{\gamma_j - \gamma_l\}]\,[\mathrm{Re}\,\{L_2(k)\}] + [\mathrm{Im}\,\{\gamma_j - \gamma_l\}]\,[\mathrm{Im}\,\{L_2(k)\}] = \frac{1}{2}(\rho_l^2 - \rho_j^2 + |\gamma_j|^2 - |\gamma_l|^2), \tag{5.1}$$

for $j, l = 1, 2, 3$. The system is guaranteed to be of full rank, under the conditions of Proposition 3.4.

Carrying out the above procedure, we obtain an approximate value for L_2 for all $k \in (c, +\infty)$. As noted in Section 3, the values of L_2 for $k \in (0, c)$ are in principle uniquely determined by analytic continuation, but for computational purposes a more specific extrapolation technique is needed. Since L_2 must be analytic for $k \in \mathbf{C}^+$ and continuous for $k \in \overline{\mathbf{C}^+}$, several possibilities are suggested by the representation formula

$$L_2(k) = L_2^{(0)}(k) \prod_j \frac{k - a_j}{k - a_j^*}. \tag{5.2}$$

Here a_j are complex constants in $\mathbf{C}^+$ corresponding to the zeros of L_2 in $\mathbf{C}^+$ and are symmetrically located with respect to the imaginary axis; the number of such zeros is either finite or countably infinite. We can obtain $L_2^{(0)}$ from $|L_2|$ for $k \in \mathbf{R}$ by one of several equivalent 'Hilbert-transform' type formulas, e.g. $L_2^{(0)}(k) = |L_2(k)|\, e^{i\phi(k)}$ with

$$\phi(k) = \frac{1}{\pi} \int_{-\infty}^{\infty} dt\, \frac{t - k}{(t - k)^2 + 0^+} \log |L_2(t)|. \tag{5.3}$$

See e.g. [20,21] and the references therein for precise statements about the validity of (5.3) and for other equivalent forms.

The zeros a_j cannot be determined from the values of $|L_2|$ on the real axis alone and must be evaluated using additional information. In order of increasing accuracy, one might consider the following possibilities:

(i) Approximate L_2 for $k \in (0,c)$ by (4.6), the reflection coefficient corresponding to $V_2(x) = c^2\, H(x)$, or by the reflection coefficient corresponding to some other potential of a particularly simple type.

(ii) Approximate L_2 by $L_2^{(0)}$ for $k \in (0,c)$. Note that this uses no information at all from the phase of L_2 for $k \in (c,+\infty)$. It will be exact if L_2 has no zeros in $\mathbf{C}^+$ and will also be fairly accurate if each $|\mathrm{Re}\, a_j|$ is much larger than c and $|\mathrm{Im}\, a_j|$, so that the product term in (5.2) is close to 1 when $k \in (0,c)$.

(iii) Approximate L_2 for $k \in (0,c)$ by determining a linear approximation to the purely imaginary function

$$\log\left(\frac{L_2(k)}{L_2^{(0)}(k)}\right) = \log\left(\prod_j \frac{k-a_j}{k-a_j^*}\right).$$

For example, in the case of generic potentials, the left-hand side should be 0 at $k=0$ and the limit as $k \to c^+$ may be easily estimated since $L_2/L_2^{(0)}$ is known for $k \in (c,+\infty)$. This method is expected to be more accurate than the second, since it uses, at least in a small way, the known phase of L_2 for $k \in (c,+\infty)$, and it will tend to produce good results providing only that $|\mathrm{Re}\, a_j|$ is larger than c and $|\mathrm{Im}\, a_j|$ for all j.

(iv) Attempt to determine some or all of the a_j in (5.2). At any particular value of $k \in (c,+\infty)$, the equation

$$\prod_j \frac{k-a_j}{k-a_j^*} = \frac{L_2(k)}{L_2^{(0)}(k)}.$$

may be thought of as a nonlinear equation for the unknowns $a_1, a_2, \ldots$, with a known right-hand side. By choosing many values of k we may hope to obtain a system of equations which may be solved, for example by nonlinear least-square methods. This method may be expected to work well if the number of zeros a_j is relatively small, or more precisely, if only a small number of them make a significant contribution to L_2 for $k \in (0, c)$.

(v) A method to recover L_2 for $k \in \mathbf{R}$ from its values for $k \in (c, +\infty)$ is derived in Section 4 of [4]. It involves evaluation of certain (singular) integrals, but no explicit analytic continuation step is required.

In practice we have found that the third method is often considerably better than the first and second, but that little or no improvement could be obtained by the fourth method. We have not at this point attempted any computations with method (v), but an exact analytical example based on this method is presented in [4]. In the next example, we illustrate the recovery of L_2 and V_2 using the three-measurement data.

Example 5.1 Figures 1-4 illustrate the use of the method based on solving (5.1) in order to recover L_2 as the intersection of three circles. Figure 1 displays a potential V_2 we would like to reconstruct, along with V_1 which has the constant value 0.7 with the support interval $x \in [-0.11, 0]$. The second known layer $\tilde{V}_1$ has the same constant value 0.7 but with the support interval $[-0.06, 0]$. The forward scattering problem was solved for $k \in (0, 100)$ on a grid with spacing $\Delta k = .025$ by the program AMPCAL which is based on certain exact solution formulas for piecewise constant potentials; such formulas are available in the literature [22]. In Figures 2-4 the exact phase of L_2 is indicated as a dashed curve obtained from the solution of the forward problem. In Figure 2 we show as a solid curve the phase of L_2 for $k \in (\sqrt{.8}, 50)$ as found from solving the linear system of equations (5.1). Since L_2 cannot be obtained as the intersection of three circles for $k \in (0, c)$, the phase of the constructed L_2 for $k \in (0, \sqrt{.8})$ in Figures 2 and 3 should be ignored. The constructed phase of L_2 for $k \in (\sqrt{.8}, 100)$ is indistinguishable from the exact phase in the scale of Figures 2 and 3.

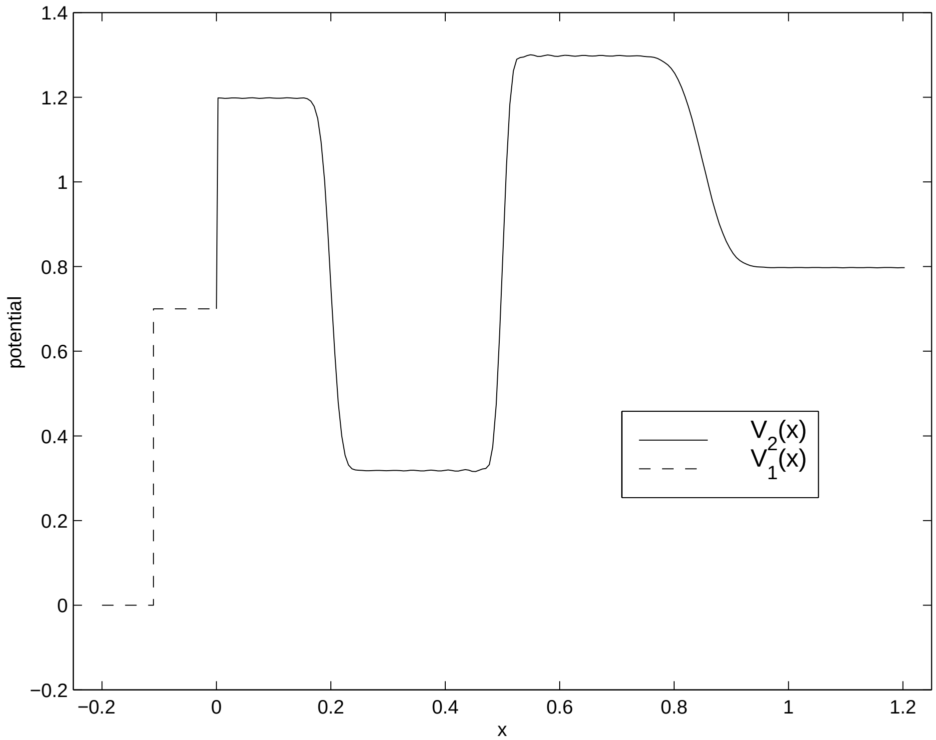

Figure 1 The potentials used in Examples 5.1 and 5.2

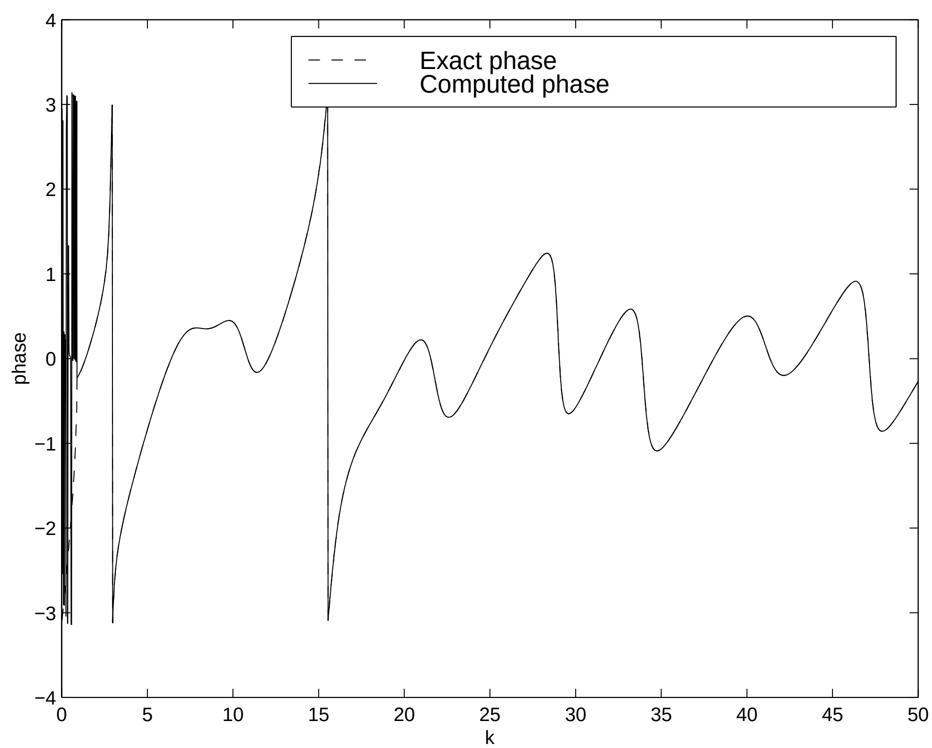

Figure 2 The exact phase of L_2 for $k \in (0, 50)$ and the computed phase for $k \in (\sqrt{.8}, 50)$

In Figure 3 we show the exact phase of L_2 on $(0,5)$ and the computed phase on $(\sqrt{.8},5)$. Finally, in Figure 4 we show the phase of L_2 on $(0,5)$ as estimated on $(0,c)$ by the extrapolation technique (iii) outlined above (for the details of of the implementation of the phase computation (5.3) we refer the reader to [23]), and we notice a good agreement with the exact phase. When this constructed phase is used with the numerical inversion method of [17], we obtain a reconstruction of V_2 which is indistinguishable from the exact V_2 on the scale of Figure 1, with a root-mean square error not exceeding 0.25%.

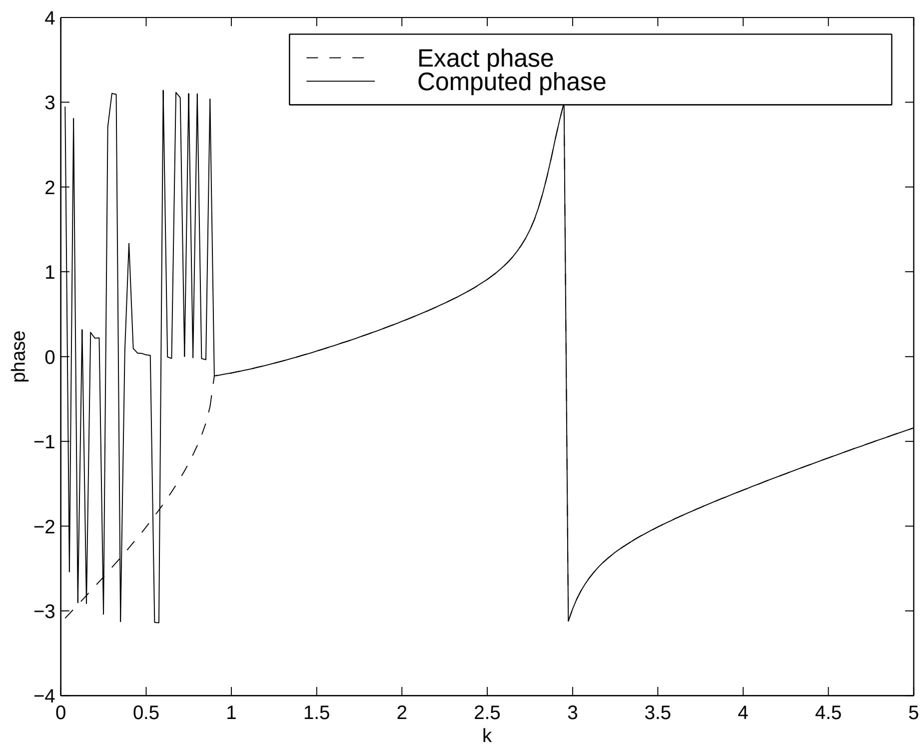

Figure 3 The exact phase of L_2 for $k \in (0,5)$ and the computed phase for $k \in (\sqrt{.8},5)$

To give an idea of how the different methods discussed above for estimating the phase for $k \in (0,c)$ compare with each other, Table 1 displays the relative percentage error in $L^2(0,c)$ for the reflection coefficient $L_2(k)$ computed by methods (i)-(iv). In this particular example the product in (5.2) contains 4 terms, so locating the a_j by the optimization indicated in method (iv) is relatively easy. However, in more complicated examples we may expect this approach to be more difficult to carry out.

Method	Error
(i)	7.3 %
(ii)	3.3 %
(iii)	0.8 %
(iv)	0.7 %

Table 1 Comparison of relative errors in L_2 as measured in $L^2(0,c)$

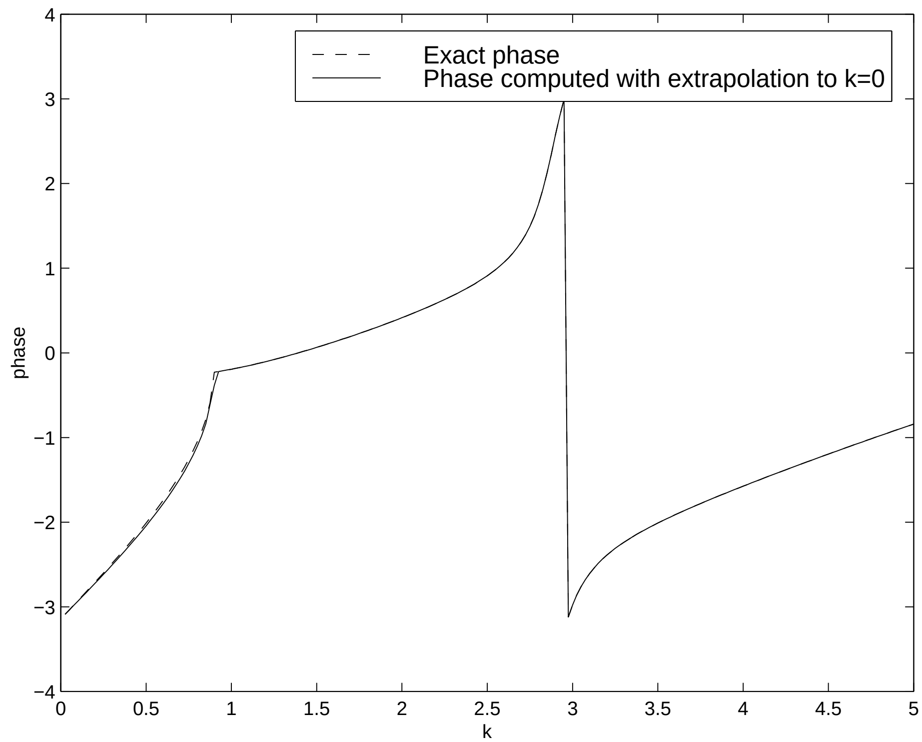

Figure 4 The exact and computed phases of L_2 for $k \in (0,5)$

In the case of two-measurement data, the procedure of finding the phase of L_2 for $k \in (c,+\infty)$ is essentially the same as in the case $c=0$, which was discussed in detail in [16]: the quantity Z in (4.4) may be computed for $k \in (c,+\infty)$ from the available scattering data, and hence F in (4.1) is known up to the sign of its imaginary part. From the behavior of Z we can estimate the location of all sign changes of $\text{Im}\{F(k)\}$ and hence determine two candidates for F, either of which is uniquely determined for $k \in (c,+\infty)$ by specifying the sign of its imaginary part at any one k value not coinciding with a zero of Z. Now one knows the behavior of $L_2(k)$ as $k \to 0$, and hence by inference the sign of $\mathrm{Im}\,\{F(k)\}$ is known on some interval $(0, k_0)$. When $c = 0$ we may use this to choose correctly between the two candidates; however, $|\mathrm{Im}\,\{F(k)\}|$ is not known for $k \in (0, c)$ when $c > 0$, and hence we cannot distinguish between the two candidates this way.

Nevertheless, for each of the two candidates for F, we may compute a corresponding guess for L_2 for $k \in (c, +\infty)$ by using (4.1), and then extrapolate to the interval $(0, c)$ by one of the methods mentioned earlier in this section. In this way, we obtain two candidates for $L_2(k)$ and seek to discard one or the other by some device. For example, we may proceed to solve the inverse scattering problem with the two choices of L_2, and typically one of the two potentials obtained this way will be unacceptable on physical grounds. Alternatively, the condition $g(t) \equiv 0$ for $t < 0$, where g defined in (4.5), may be checked.

Example 5.2 Using the two-measurement data $\{V_1, |L_2|, |L|\}$ from Example 5.1, we find that one of the two candidates for L_2 does not satisfy (4.5) and hence can be eliminated, leaving the correct solution as the only other possibility. The reconstructed L_2 and reconstructed V_2 based on the use of the two-measurement data are indistinguishable from reconstructed quantities based on the use of the three-measurement data and hence agree well with the exact quantities.

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