JOURNAL OF COMPUTATIONAL PHYSICS 112, 273–281 (1994)

Use of Partial Knowledge of the Potential in the Phase Problem of Inverse Scattering

MICHAEL V. KLIBANOV

Department of Mathematics, University of North Carolina at Charlotte, Charlotte, North Carolina 28223

AND

PAUL E. SACKS

Department of Mathematics, Iowa State University, Ames, Iowa 50010

Received February 1, 1993

We consider the problem of determining a potential $V(x)$ in the one-dimensional Schrödinger equation, given as data the reflectivity $r(k) = |R(k)|^2$, where $R(k)$ denotes the usual quantum mechanical reflection coefficient. It is well known that in the absence of phase information, there can be a considerable degree of nonuniqueness, which is closely connected to the presence of zeros of $R(k)$ in the upper half of the complex plane. Some earlier work of the authors showed that this ambiguity can be resolved by providing a small amount of extra information about the potential. In this article we develop a computational technique, based on an optimization approach to the problem of locating the zeros of $R(k)$. Some numerical examples are given.

INTRODUCTION

Let $V(x)$ be a real-valued potential on $\mathbb{R}$ with $V(x) \equiv 0$ for $x < 0$ and decaying in a suitable fashion as $x \to +\infty$. The Schrödinger equation

$$\phi'' + (k^2 - V(x))\,\phi = 0, \qquad -\infty < x < \infty, \tag{1.1}$$

then has the solution

$$\begin{aligned} \psi(x, k) &= e^{ikx} + R(k)\, e^{-ikx}, && x < 0, \\ &\sim T(k)\, e^{ikx}, && x \to +\infty, \end{aligned} \tag{1.2}$$

where $R(k)$, $T(k)$ are reflection and transmission coefficients. We are concerned with the following inverse scattering problem

Determine the potential $V(x)$ assuming that the reflection amplitude $r(k) = |R(k)|^2$ is known.

This problem is of central importance, for example, in neutron and X-ray reflectivity studies. See [5] for the proceedings of a recent conference on this topic.

It is well known that if the potential has no bound states then it is uniquely determined by $R(k)$. However, the absence of phase information introduces considerable ambiguity, which is directly connected with the presence of zeros of $R(k)$ in the upper half of the complex plane. These zeros are the *fundamental* obstacle to unique recovery of the potential, in the sense that they encode all of the information about the potential which is present only in the phase of $R(k)$. Any method for recovery of V must implicitly or explicitly locate these zeros, by using some kind of extra information about the potential. In our case the extra data will consist of *partial knowledge of the potential.* The fact that this kind of information can compensate for the lack of phase data was proven in [8]. Here our main goal is to investigate a computational algorithm for reconstruction of a potential $V(x)$, given the reflection amplitude r and partial knowledge of V. See also [11, 5] for some previous work on this problem. It is closely related to the so-called phase problem of optics, namely the determination of a function from the modulus of its Fourier transform, see, e.g., [1, 6, 7].

Recall that the Sobolev space $W^{k,p}(\Omega)$ consists of functions having derivatives up through order k belonging to $L^p(\Omega)$. We need also the weighted L^1 space

$$L_2^1(\mathbb{R}) = \left\{ f : \int_{-\infty}^{\infty} |f(x)|\,(1 + x^2)\,dx < \infty \right\}. \tag{1.3}$$

Let us define the class of potentials

$$\begin{aligned} \mathscr{A} = \{ V \in L_2^1(\mathbb{R}) \cap W^{1,1}(0, \infty) &: V(x) \equiv 0 \\ &\text{for } x < 0,\ V \text{ has no bound states} \}. \end{aligned} \tag{1.4}$$

581/112/2-5

0021-9991/94 $6.00

The no bound state condition is satisfied, for example, if $V(x) \geqslant 0$ which holds in many cases of practical interest.

As remarked earlier, we may hope that unique recovery of the potential is possible, provided certain extra information about the potential is given; i.e., the class of admissible solutions is suitably restricted. The following theorem of this type was proved in [8].

THEOREM 1. *Assume that* $V \in \mathscr{A}$, $V_0 = \lim_{x \to 0+} V(x) \neq 0$ *and* $R(k)$ *has no real zeros of infinite order. Fix* $\varepsilon > 0$. *Then* $R(k)$ *is uniquely determined for all real* k *by* $r(k)$ *and* $\{V(x): 0 < x < \varepsilon\}$. *In particular* $V(x)$ *is uniquely determined for* $x > \varepsilon$ *by* $r(k)$ *and* $\{V(x): 0 < x < \varepsilon\}$.

We now consider some ideas for numerical solution of the problem whose uniqueness is guaranteed by Theorem 1.

Let us define the mapping T by

$$T(V) = r, \tag{1.5}$$

where $r(k) = |R(k)|^2$ is the reflection amplitude corresponding to the given potential V. For a given reflection amplitude r and function $V_0 = V_0(x)$ defined for $0 < x < \varepsilon$, define the sets of potentials

$$\Sigma(r) = \{V \in \mathscr{A}: T(V) = r\} \tag{1.6}$$

and

$$\Gamma(V_0) = \{V \in \mathscr{A}: V(x) \equiv V_0(x), 0 < x < \varepsilon\}. \tag{1.7}$$

The content of Theorem 1 is that the solution V is the unique point of intersection of the sets $\Sigma(r)$ and $\Gamma(V_0)$. To obtain the solution numerically there are two natural optimization approaches we might consider,

$$\min_{V \in \Sigma(r)} \|V - V_0\| \tag{1.8}$$

and the dual problem

$$\min_{V \in \Gamma(V_0)} \|T(V) - r\| \tag{1.9}$$

for suitable norms $\|\cdot\|$. In either case it is clear that if the data (r, V_0) is consistent, i.e., corresponds to a potential $V \in \mathscr{A}$, then the exact potential V is the unique solution.

We will focus here on the first formulation, the minimization problem (1.8). Some study of (1.9) will appear elsewhere. The principal advantage of (1.8) is that the constraint set $\Sigma(r)$ is in a certain sense much smaller than $\Gamma(V_0)$, so that in computing a solution of (1.8) only a relatively small parameter space needs to be searched.

FORMULATION OF AN OPTIMIZATION PROBLEM

For convenience, we will replace the minimization problem (1.8) by an equivalent one in which the potential V is replaced by its "impulse response function" $g = g(t)$, defined by

$$g(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} R(k)\, e^{-ikt}\, dk \tag{2.1}$$

so that

$$R(k) = \int_{-\infty}^{\infty} g(t)\, e^{ikt}\, dt =: \hat{g}(k). \tag{2.2}$$

It is known that the potential V on any interval $[0, X]$ determines the impulse response function $g(t)$ on $[0, 2X]$ and conversely. More precisely, g and V are related by the fact that $g(t) = u(0, t)$, where $u = u(x, t)$ is the unique solution of the Goursat problem

$$u_{tt} - u_{xx} + V(x)\, u = 0, \qquad 0 < x < t, \tag{2.3}$$

$$u_x(0, t) - u_t(0, t) = 0, \qquad 0 < t, \tag{2.4}$$

$$u(x, x) = \tfrac{1}{2} \int_0^x V(s)\, ds, \qquad 0 < x. \tag{2.5}$$

The fact that g is determined on $[0, 2X]$ by V on $[0, X]$ is a domain of dependence property, which may be proved by standard energy estimates, while the reverse implication is a result of time domain inverse scattering theory; see, e.g., [10].

Thus we may regard $g(t)$ as the unknown function to be determined, in place of $V(x)$, and we assume that $g(t)$ is equal to a known function $g_0(t)$ for $0 < t < 2\varepsilon$.

We now consider

$$\min_{h \in \sigma(r)} \|h - g_0\|_{L^2(0, 2\varepsilon)}, \tag{2.6}$$

where

$$\sigma(r) = \{h \in \mathscr{B}: |\hat{h}(k)|^2 = r(k)\} \tag{2.7}$$

and

$$\mathscr{B} = \{h: V \in \mathscr{A}\} \tag{2.8}$$

is the set of impulse responses corresponding to potentials in $\mathscr{A}$. This problem has a unique solution, for consistent data, according to the previous discussion.

The following is also proved in [8].

THEOREM 2. *Assume the hypotheses of Theorem* 1. *If* $h \in \sigma(r)$ *then there exists a function* $a(t)$ *with support in* $[0, \infty)$ *such that*

$$h(t) = G(t) + (G * a)(t)$$
$$= G(t) + \int_0^t a(s)\, G(t-s)\, ds, \tag{2.9}$$

where

$$\hat{G}(k) = \sqrt{r(k)}\, e^{i\phi(k)} \tag{2.10}$$

$$\phi(k) = -\pi + \lim_{r \to +\infty} \lim_{\delta \to 0+} \frac{1}{2\pi} \times \int_{\delta < |k-\xi| < r} \frac{\log(r(\xi))}{k-\xi}\, d\xi, \qquad r(k) \neq 0, \tag{2.11}$$

and

$$\hat{a}(k) = \prod_{j=1}^{n} \frac{k-a_j}{k-\bar{a}_j} - 1 \tag{2.12}$$

with constants $a_1, a_2, \ldots, a_n$ *in the upper half plane. That is to say,*

$$\hat{h}(k) = \hat{G}(k) \prod_{j=1}^{n} \frac{k-a_j}{k-\bar{a}_j}. \tag{2.13}$$

The point of Theorem 2 is to exhibit an explicit representation of the set $\sigma(r)$; namely it may be parameterized by the set of all finite sequences $a_1, a_2, \ldots, a_n$ of complex numbers in the upper half plane, which we see are the zeros of the Fourier transform $\hat{h}$.

At this point one might consider the following approach. Substitute $h = g_0$ in the left side of (2.9), and then solve for $a(t)$ on $[0, 2\varepsilon]$. The function $a(t)$ is analytic and hence is uniquely determined for all $t > 0$. Therefore $g(t)$ and subsequently $V(x)$ may be found. The difficulty with this approach, of course, is that recovery of $a(t)$ for $t > 2\varepsilon$ amounts to an analytic continuation step, which we may expect to be very unstable. This difficulty will be especially severe when ε is small, because then the computed solution $a(t)$ will tend to be more inaccurate.

It seems preferable, therefore, to take a different point of view, namely to focus on the recovery of the Fourier transform $\hat{a}$, instead of a itself, that is to seek to determine the a_j's in (2.12). In this way we are able to exploit the fact that we have considerable a priori information about a, through the form of its Fourier transform. In particular the problem becomes finite dimensional (albeit with the dimension itself as one of the unknowns) and no analytic continuation step will be required. The main disadvantage is that the computational problem becomes nonlinear. As long as n is not so large, as often happens in practice, this difficulty does not seem so serious.

DESCRIPTION OF THE ALGORITHM

To proceed, let us define $\sigma_n(r)$ to be the set of all $h \in \mathscr{B}$ such that

$$\hat{h}(k) = \hat{G}(k) \prod_{j=1}^{n} \frac{k-a_j}{k-\bar{a}_j} \tag{3.1}$$

for some $a_1, \ldots, a_n$ with $\operatorname{Im} a_j \geq 0$ and G as in (2.10). Terms with a_j on the real axis make no contribution, but it is convenient to allow the a_j's to vary over the closed upper half plane. Also let $\sigma_0(r) = \{G\}$. Then

$$\sigma_n(r) \subset \sigma_{n+1}(r), \qquad \sigma(r) = \bigcup_{n=0}^{\infty} \sigma_n(r). \tag{3.2}$$

Each $\sigma_n(r)$ may be thought of as a $2n$ real dimensional submanifold of $\mathscr{B}$. If the exact solution g is such that $\hat{g} = R$ has N zeros in the upper half plane, then

$$g \in \sigma_n(r), \qquad n \geq N, \tag{3.3}$$

and the minimization problem

$$\min_{h \in \sigma_n(r)} \|h - g_0\|_{L^2(0, 2\varepsilon)} \tag{3.4}$$

has the unique solution g for $n \geq N$ with zero residual, while for $n < N$ the residual is strictly positive at any solution of (3.4).

Thus we can obtain the solution g by solving (3.4) for any sufficiently large n. In practice it is clearly to our advantage to have n as close to N as possible, in order to keep down the size of the parameter space, and also to reduce the possibility of local minima of the objective functional which are not true solutions. Thus we might just solve (3.4) starting with $n = 0$ and then increase n until a zero residual is found.

Consider now the minimization problem (3.4) for a fixed value of $n > 0$ (the $n = 0$ case being trivial). For $h \in \mathscr{B}$ we must have $\hat{h}(k) = \bar{\hat{h}}(-\bar{k})$ so that if a_j occurs in the representation (2.12), so does $-\bar{a}_j$. In all cases of interest to us (e.g., if $V(x) \geq 0$) the exact solution must satisfy $\hat{g}(0) = R(0) = -1$ from which we may conclude that the number of a_j's on the imaginary axis must be even.

For simplicity let us actually consider the "generic" case that (i) no a_j lies on the imaginary axis, and (ii) no a_j is repeated. In this case $\sigma_n(r)$ effectively depends on n real parameters, which we may regard as the real and imaginary parts of the $n/2$ roots in the positive quadrant. The

remaining cases could be handled as special limiting situations. With these assumptions one may derive the following explicit form for $a(t)$ in terms of the zeros of $\hat{a}+1$, namely,

$$a(t)=\sum_{l=1}^{n} b_l e^{-i\bar{a}_l t}, \qquad t\geq 0, \tag{3.5}$$

$$b_l=-2\,\mathrm{Im}\, a_l \prod_{j\neq l}\frac{\bar{a}_l-a_j}{\bar{a}_l-\bar{a}_j}. \tag{3.6}$$

Substitution of (2.9)–(2.12) and (3.5)–(3.6) into (3.4) will yield a nonlinear finite dimensional minimization problem.

If we can obtain the correct values $a_1 \cdots a_n$, then $R(k)$ and consequently $V(x)$ may be found. In the next section we discuss each step in more detail.

We conclude this section with some remarks about continuous dependence of the solution on the data. If we are interested in recovering the potential on an interval $[0, X]$, then the "condition number" (i.e., the factor by which relative error in the data is magnified in the solution) clearly depends in some manner on ε, varying from ∞ to 1 as ε varies from 0 to X. It also must depend on certain features of the potential being computed. Roughly speaking, if the potential has little complexity for $0<x<\varepsilon$, but more complexity away from $x>\varepsilon$, it will be a more ill-conditioned situation, than when the reverse is true. We may also expect the conditioning to degenerate as N (the number of complex zeros of R) increases.

SUMMARY AND EXAMPLES

We now summarize the steps in our algorithm for computing the potential V. Recall that the given data is the reflectivity $\{r(k): k>0\}$ and initial segment of the potential $\{V(x): 0<x<\varepsilon\}$.

Step 1. Compute $\phi(k)$.

Step 2. Compute $\hat{G}(k)$.

Step 3. Compute $G(t)$.

Step 4. Compute $g(t)$ for $0<t<2\varepsilon$.

Step 5. Compute N and the zeros $a_1 \cdots a_N$.

Step 6. Compute $\hat{g}(k)=R(k)$ for $k>0$.

Step 7. Compute the potential $V(x)$ for $x>0$.

We now discuss each of these steps in turn.

Step 1. The phase function $\phi(k)$ may in principle be computed using the integral formula (2.11). To avoid difficulties with limits, the following alternative formula may be used [8, Eq. (5.1)],

$$\phi(k)=-\pi+\frac{1}{2\pi}\int_{-1}^{1}\log\left[\frac{r(k)\,r(1/\xi)}{r(k+\xi)\,r(k+1/\xi)}\right]\frac{d\xi}{\xi}, \tag{4.1}$$

as long as $r(k)\neq 0$. The integrand in (4.1) has a removable singularity at $\xi=0$, with the limiting value being $\frac{1}{2}(r'(k)/r(k))-2k$. Thus $\phi(k)$ may be evaluated by any convenient quadrature routine. We remark that the accuracy is improved by substituting the asymptotic form $r(k)\sim(V_0/4k^2)^2$ (cf. (2.10) of [8]) for large k.

Step 2. We obtain $\hat{G}(k)$ directly from (2.10).

Step 3. One may compute the inverse Fourier transform $G(t)$ with a standard FFT routine. We remark that since $G(t)$ is real and vanishing for $t<0$, it may also be obtained as the cosine transform of $\mathrm{Re}\,\hat{G}(k)$ or the sine transform of $\mathrm{Im}\,\hat{G}(k)$. Depending on the situation, one of these may produce far more accurate results than the other, and so it will also be more accurate than the standard FFT which is the average of these two. For potentials in the class $\mathscr{A}$ it will generally be the sine transform of $\mathrm{Im}\,\hat{G}(k)$ which is more accurate. See [9] for more discussion of this point.

Step 4. If V is given on $[0, \varepsilon]$, the impulse response function $g(t)$ may be determined as $g(t)=u(0, t)$, where $u=u(x, t)$ is the unique solution of (2.3)–(2.5), which is solvable in a straightforward way by finite difference techniques. See, e.g., [9].

Step 5. The zeros $\{a_1 \cdots a_N\}$ are obtained by solving a finite sequence of minimization problems. We now describe explicitly the functions to be minimized. Fix an even integer $n\geq 2$ and let $m=n/2$. Set $\gamma=(\alpha, \beta)$, where $\alpha=(\alpha_1, ..., \alpha_m)$, $\beta=(\beta_1, ..., \beta_m)$, so that $\alpha, \beta\in\mathbb{R}^m$ and $\gamma\in\mathbb{R}^n$. We think of $\alpha_j+i\beta_j=a_j$ as a typical zero of $\hat{a}+1$ in the upper half plane, so actually we restrict β to lie in $\mathbb{R}^m_+=\{\beta\in\mathbb{R}^m: \beta_j\geq 0,\ j=1, ..., m\}$. Recall that if $\alpha_j+i\beta_j$ is a zero, so is $-\alpha_j+i\beta_j$. Thus we could restrict α to lie in $\mathbb{R}^m_+$ also, but it seems more convenient not to do so. Define $\mathbb{R}^n_+=\{\gamma=(\alpha, \beta)\in\mathbb{R}^m\times\mathbb{R}^m_+\}$. According to Theorem 2, any $h\in\sigma_n(r)$ is completely specified by the vector γ.

Now for any $\gamma\in\mathbb{R}^n_+$, set

$$J(\gamma)=\|h-g_0\|^2_{L^2(0,2\varepsilon)}=\|G-g_0+a*G\|^2_{L^2(0,2\varepsilon)}, \tag{4.2}$$

where

$$\hat{a}(k)=\prod_{j=1}^{n}\frac{k-a_j}{k-\bar{a}_j}-1,$$

$$a_j=\alpha_j+i\beta_j, \qquad a_{n+1-j}=-\alpha_j+i\beta_j, \qquad j=1, ..., m. \tag{4.3}$$

With g_0 and G fixed, (4.2) depends only on γ. The convolution term $a*G$ may be explicitly evaluated using (3.5)–(3.6).

A minimum of J over $\mathbb{R}^n_+$ corresponds to a solution $g=G+a*G$ of the minimization problem (3.4). Since it is more convenient computationally to work with an unconstrained minimization problem, we extend J to all of $\mathbb{R}^n$, in such a way that the minimum is unlikely to be found

outside of $\mathbb{R}^n_+$. First, we note that $a(t)$ is already defined for any $\gamma \in \mathbb{R}^n$ by formulas (3.5)–(3.6) (even though (2.12) only defines a if $\gamma \in \mathbb{R}^n_+$), and we can try to ensure that a (local) minimum of J only takes place for $\gamma \in \mathbb{R}^n_+$ by redefining

$$J(\gamma) = \|G - g_0 + a * G\|^2_{L^2(0,2\varepsilon)} + \lambda\, |\beta_-|^2. \tag{4.4}$$

Here λ is a positive parameter, $|\cdot|$ is the Euclidean norm on $\mathbb{R}^m$, and $\beta_- \in \mathbb{R}^m$, is the negative part of β; i.e., $(\beta_-)_i = -\min(0, \beta_i)$. It is not crucial what value of λ is chosen, since if we ever obtain a minimum of J with some component of β being negative, we know that this is an inadmissible solution, and we simply repeat the calculation with a larger value of λ. In all the cases that we tried it was sufficient to take $\lambda = 1$. By convention, we will say that for $n = 0$, J is the constant $\|g_0 - G\|^2_{L^2(0,2\varepsilon)}$.

The zeros are now obtained as follows. For $n = 0, 2, 4, \ldots$ until satisfied, we minimize J over $\mathbb{R}^n$ using convenient optimization software, noting the residual value of J at the minimizer. We stop when a zero residual is obtained, or in practice when no decrease of the residual is obtained by increasing n. Rearrangement of the minimizing vector γ yields the desired zeros $\{a_1 \cdots a_N\}$.

In the examples below, the minimization was done using the MINPACK routine **lmdif**, which computes the gradient of J by finite differencing. It would clearly be possible to obtain analytic expressions for the partial derivatives of J, if more speed were required. We remark also that even though the minimization is in principal over all of $\mathbb{R}^n$, the objective function J appears to be highly coercive, so that all of the action really takes place in a fairly limited region of $\mathbb{R}^n$. Nevertheless multiple local minima are still a possibility, so that several different choices of initial guess should be tried.

Step 6. Once $a_1, \ldots, a_N$ have been found, we obtain directly

$$R(k) = \hat{g}(k) = \hat{G}(k) \prod_{j=1}^{N} \frac{k - a_j}{k - \bar{a}_j}. \tag{4.5}$$

Step 7. With the full complex reflection coefficient $R(k)$ now available, the procedure for recovery of $V(x)$ is classical, e.g., [3, 4]. The numerical procedure we actually used in the examples shown below, based on (2.1)–(2.5), is taken from [9].

To illustrate this algorithm with an example, consider the potential $V(x)$ shown in Fig. 1.

The wave function ψ in (1.2) may be easily computed by a standard ODE solver, using the conditions that $\psi(x, k) = T(k)\, e^{ikx}$ for $x > 1$ and that ψ, ψ' are continuous. We thus obtain the reflectivity $r(k)$ which is shown in Fig. 2 on a logarithmic scale. We actually use $r(k)$ sampled at points $k = 0.025 * j$, $j = 1, \ldots, 2000$. We now follow steps 1–7 described above. The phase function ϕ is computed from (4.1), and we obtain $\hat{G}(k)$ directly. Recall that $\hat{G}(k)$ is the reflection coefficient for a potential V^* which has exactly the same reflectivity $r(k)$ as V, but with no zeros in the upper half plane. The difference between the two potentials, representing the information about V contained only in the phase of $R(k)$, is considerable, as is shown in Fig. 3.

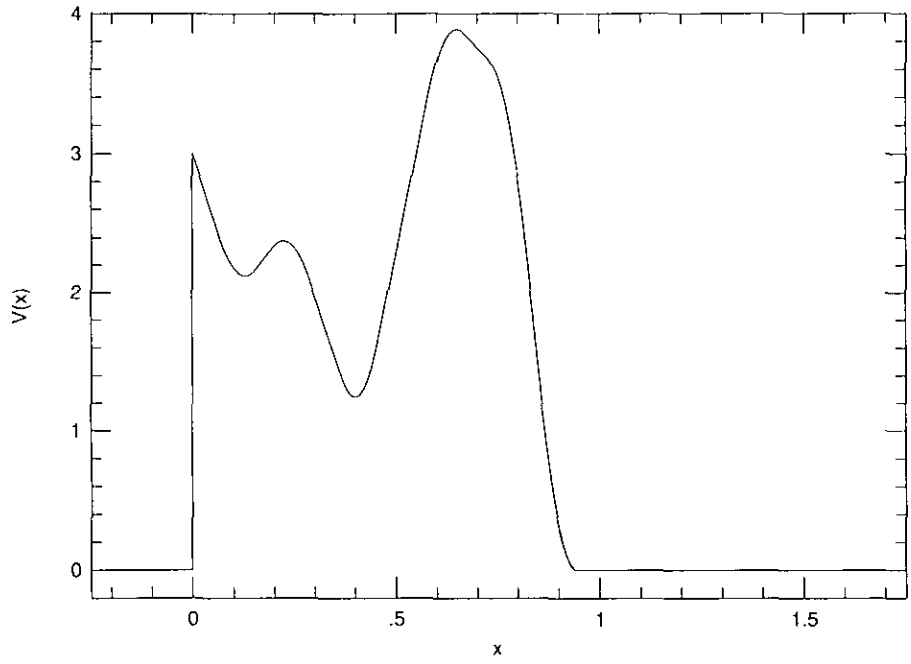

FIG. 1. The exact potential to be reconstructed.

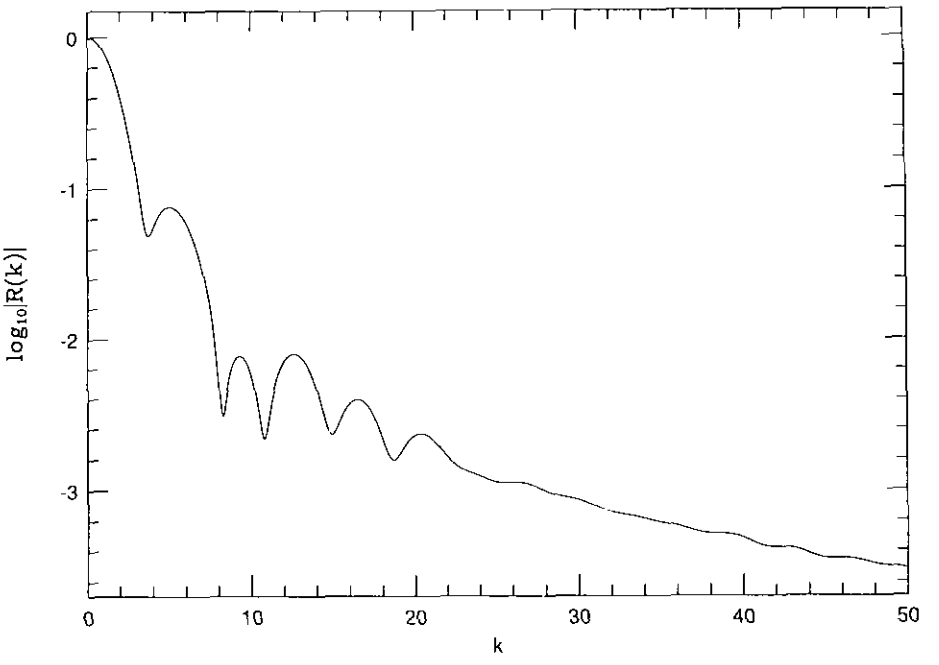

FIG. 2. The reflection amplitude for the potential of Fig. 1.

We now come to the central task, which is to estimate the zeros of $R(k)$. We will take $\varepsilon = 0.3$, and in Fig. 4 we show the two impulse response functions g, G, obtained in steps 3 and 4, on the corresponding time interval $[0, 0.6]$. Carrying out the procedure described in Step 5, we obtain the following residual values:

$$\min J = 4.1 \times 10^{-3} \quad \text{for} \quad n = 0,$$
$$\min J = 7.7 \times 10^{-7} \quad \text{for} \quad n = 1,$$
$$\min J = 1.4 \times 10^{-9} \quad \text{for} \quad n = 2,$$
$$\min J = 1.4 \times 10^{-9} \quad \text{for} \quad n = 3.$$

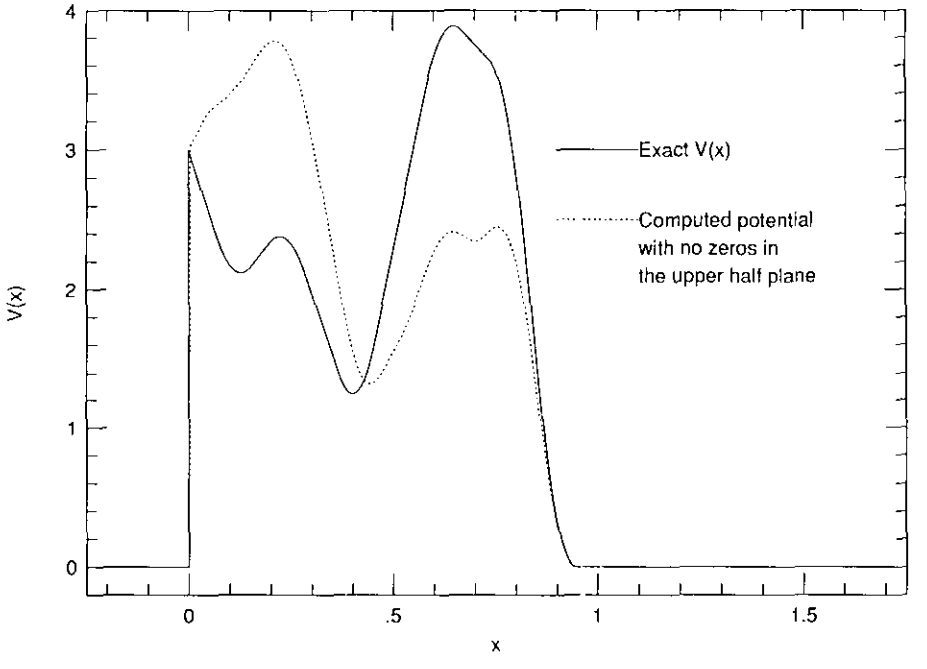

FIG. 3. The exact potential V shown with the potential V^* having the reflection coefficient $\hat{G}(k)$. Thus V, V^* have the same reflection amplitude, but the reflection coefficient of V^* has no zeros in the upper half plane.

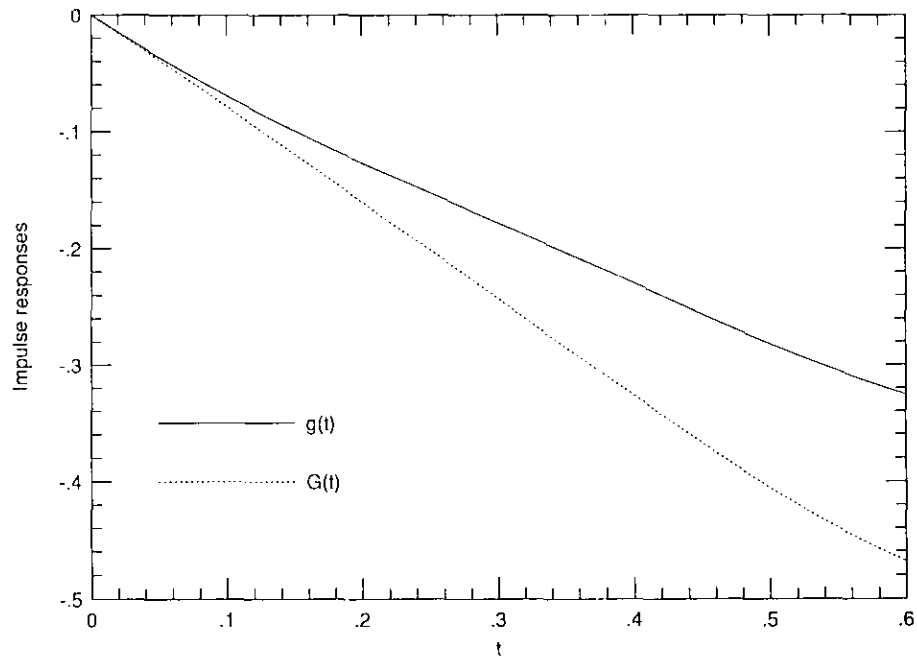

FIG. 4. The impulse responses g, G for V, V^*, respectively, on the time interval $[0, 0.6]$.

The apparent result, therefore, is that $N=4$ and the two zeros found in the first quadrant are $a_1 \approx 3.668 + 0.4309i$ and $a_2 \approx 8.267 + 0.2062i$. Finally we substitute these values into (4.5) to obtain the full complex reflection coefficient and obtain the potential $V(x)$ shown in Fig. 5, by the method of [9]. In Fig. 6 we show the final reconstruction of V using the slightly smaller value of $\varepsilon = 0.25$. As we decrease ε further, the accuracy of the reconstruction begins to degenerate quite rapidly.

SOME GENERALIZATIONS

Some weakening of the conditions we have imposed on the potential is possible. A case of special interest (e.g., [5])

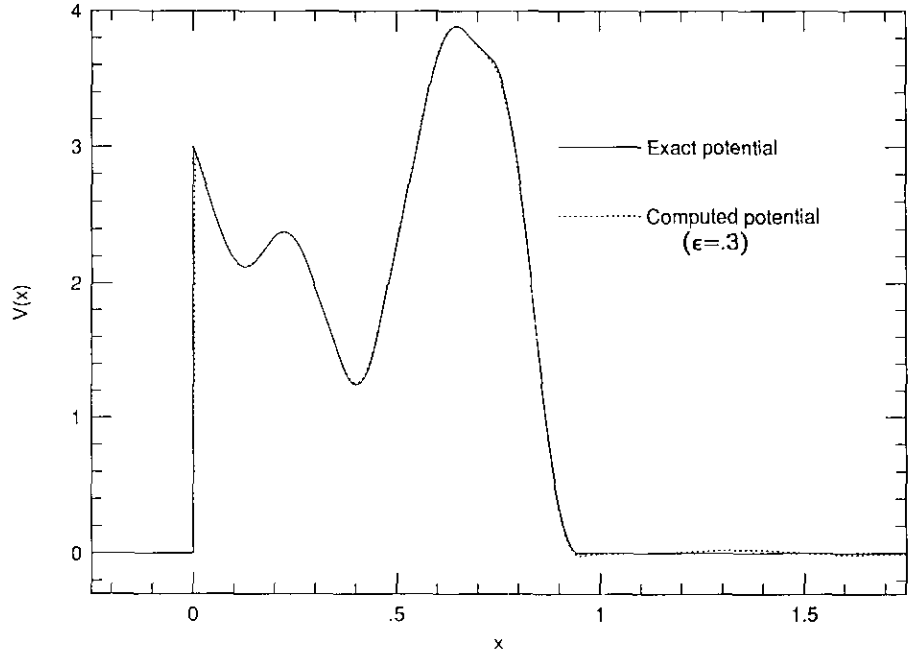

FIG. 5. Reconstruction of the potential V using $\varepsilon = 0.3$.

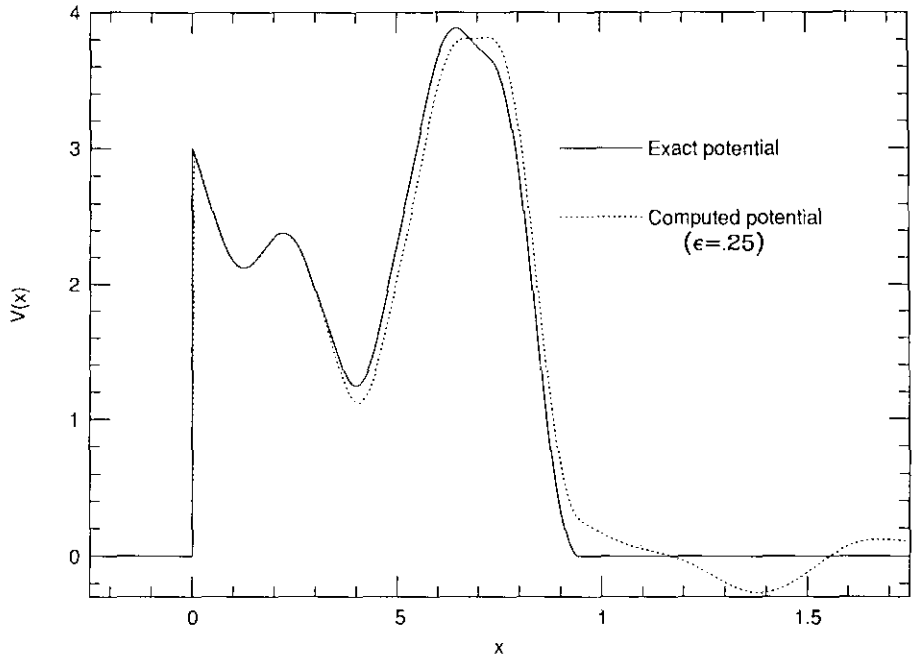

FIG. 6. Reconstruction of the potential V using $\varepsilon = 0.25$.

is when the potential is not decaying at $+\infty$, but instead $\lim_{x \to +\infty} V(x) = V_0 > 0$. It is necessary to suitably modify the definition of scattering data; for example, in (1.2) we must have

$$\psi(x, k) \sim e^{i\sqrt{k^2 - V_0}\, x}, \qquad x \to +\infty,$$

where $\sqrt{k^2 - V_0}$ is understood to be $i\sqrt{V_0 - k^2}$ for $k^2 < V_0$. See, e.g., [2] for a thorough treatment of inverse scattering for such potentials, and [9] for a computational method.

For this class of potentials, the previous discussion remains valid *formally*, but we have not been able to give a rigorous proof of Theorems 1 and 2 in all respects. Numeri-

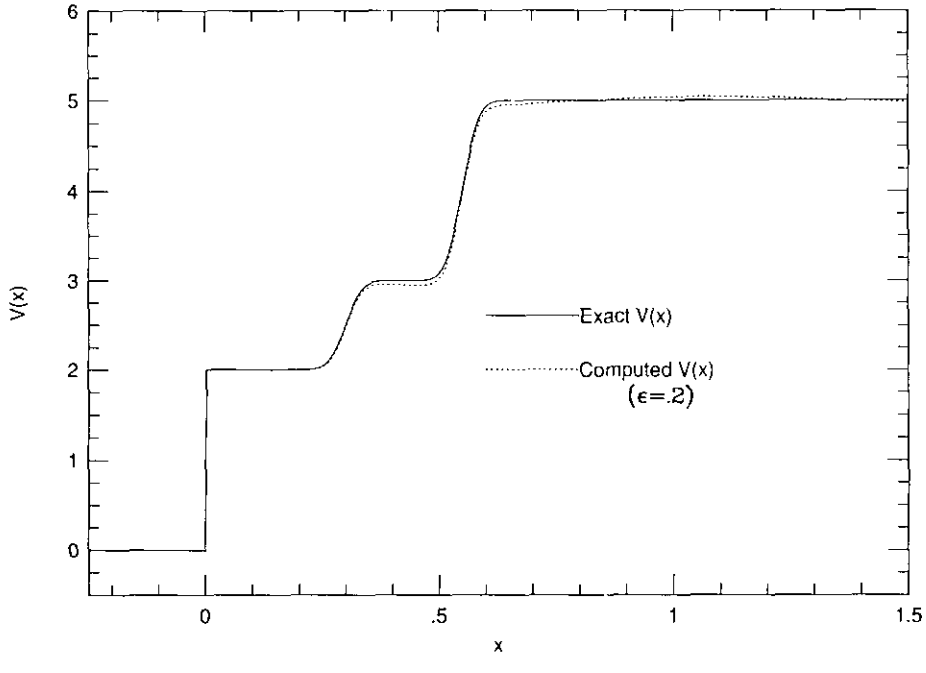

FIG. 7. Reconstruction of a nondecaying potential, using $\varepsilon = 0.2$.

cal evidence strongly suggests that the algorithm we are proposing here is a valid one for this larger class of potentials. Figure 7 shows the reconstruction of a "three-layer" potential, for which the corresponding reflection coefficient turns out to have one pair of zeros in the upper half plane.

Another generalization consists in replacing the jump condition on $V(x)$ at $x=0$ by a jump condition on some derivative of V. For example, we might assume that $V(0+)=0$, $V_1=\lim_{x\to 0+} V'(x)\neq 0$, and $V\in W^{2,1}(0,\infty)$. See Section 3 of [8] for some more discussion.

ESTIMATING THE VALUE OF N

The key step 5 in the algorithm would be simplified somewhat if the value of N, the number of terms in the product of (4.5), were known, or approximately known. We cannot expect this value to depend in any sense continuously on the potential, since it is integer valued. Nevertheless, it will often be the case that the value of N for the unknown potential V will be the same as that for some nearby "reference potential" V^*. Thus it may be of some value to be able compute the number N for a given potential V. This would not be very feasible if it were necessary to compute $R(k)$ for many values of k in the upper half plane, but it turns out that there is an easy alternative, resulting from a relationship between zeros of $R(k)$ in the upper half plane and the behavior of $R(k)$ on the real axis. Specifically, the number of zeros of $R(k)$ in $\{\operatorname{Im} k>0\}$ is directly related to the net change of $\arg(R(k))$ on the real axis, that is, the number of times $R(k)$ winds around the origin of the complex plane as k goes from $-\infty$ to $+\infty$.

If F is any continuous complex valued function on $\mathbb{R}$ with $F(k)\neq 0$ for any $k\in\mathbb{R}$, define

$$W(F)=\frac{1}{2\pi}(\arg F)\Big|_{k=-\infty}^{k=+\infty},$$

where $\arg(\cdot)$ refers to any continuous (multivalued) determination of the argument. That is, $W(F)$ is the net increase in $\arg F(k)$ along the real axis divided by 2π, which is the definition of the winding number.

Integrating R'/R along the real axis with contour closed in the upper half plane, making use of the classical argument principle and the asymptotic behavior $R(k)\sim V_0/4k^2$ as $k\to\infty$ in the upper half plane, we obtain

LEMMA. *Let V satisfy the hypotheses of Theorem 1, assume that R has no real zeros, and let N be the number of zeros of the reflection coefficient $R(k)$ in the upper half plane. Then $N=W(R)-1$.*

This result is somewhat analogous to Levinson's theorem, which states a relationship between the number of bound states of a potential, which is equal to the number of zeros of $1/T(k)$ in the upper half plane and the winding number $W(1/T)$.

CONCLUSIONS

We have proposed an algorithm for the numerical determination of the potential $V(x)$ in a one-dimensional Schrödinger equation, using as data $r(k)=|R(k)|^2$, the amplitude of the complex reflection coefficient, and partial knowledge of the potential, $\{V(x): 0<x<\varepsilon\}$. In typical cases, recovery of the phase involves the solution of a nonlinear optimization problem in a relatively low dimensional parameter space. We presented numerical examples showing effective reconstruction of the potential.

ACKNOWLEDGMENTS

Research of the first author was supported by the Office of Naval Research under Contract N0014-92-J-1008. Research of the second author was supported by the National Science Foundation under Contract DMS-9201936. The first author would like to thank A. V. Tikhonravov for helpful discussions.

REFERENCES

1. R. E. Burge, M. A. Fiddy, A. H. Greenaway, and G. Ross, *Proc. R. Soc. London A* **350**, 191 (1976).
2. A. Cohen and T. Kappeler, *Indiana Univ. Math. J.* **34**, 127 (1985).
3. K. Chadan and P. Sabatier, *Inverse Problems in Quantum Scattering Theory* (Springer-Verlag, New York, 1989).
4. L. D. Faddeev, *Am. Math. Soc. Transl.* **65**, 129 (1967).
5. G. Felcher and T. Russell (Eds.), *Phys. B* **173**, (1991).
6. N. E. Hurt, *Phase Retrieval and Zero Crossings* (Kluwer, Dordrecht, 1989).
7. M. Klibanov, *Sov. Math. Dokl.* **32**, 668 (1985).
8. M. Klibanov and P. E. Sacks, *J. Math. Phys.* **33**, 3813 (1992).
9. P. E. Sacks, *Wave Motion* **18**, 21 (1993).
10. W. W. Symes, *J. Math. Anal. Appl.* **94**, 435 (1983).
11. A. V. Tikhonravov, *USSR Comput. Math. Math. Phys.* **25**, 77 (1985).