

RECONSTRUCTION OF STEPLIKE POTENTIALS

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ABSTRACT. In this article we study some numerical methods for the determination of a potential $V(x)$ in the one dimensional Schrödinger equation. We assume that $V(x) = 0$ for $x < 0$, and tends to a nonnegative constant as x tends to positive infinity. We suppose also that there are no bound states. The approach pursued here is based on a transformation to an equivalent ‘time domain’ problem, namely the determination of an unknown coefficient in a wave equation. We also discuss some advantages of replacing the unknown potential by an equivalent unknown impedance.

1. INTRODUCTION

In this article we study some numerical methods for the one-dimensional inverse scattering problem of quantum mechanics, namely the determination of a potential $V(x)$ from reflection data. Motivated by applications in neutron reflectivity ([1],[2]), we consider potentials of the following special form:

$$V(x) \equiv 0 \quad x < 0 \quad \lim_{x \rightarrow \infty} V(x) = V_\infty \quad (1.1)$$

where $V_\infty \geq 0$ is a constant.

For such a potential, there exist solutions of the time reduced Schrödinger equation

$$\psi'' + (k^2 - V(x))\psi = 0 \quad -\infty < x < \infty \quad (1.2)$$

in the form

$$\begin{aligned} \psi = \psi(x, k) &= e^{ikx} + R(k)e^{-ikx} \quad x < 0 \\ &\sim T(k)e^{i\theta(k)x} \quad x \rightarrow +\infty \quad \theta(k) = \sqrt{k^2 - V_\infty} \end{aligned} \quad (1.3)$$

Here $\theta(k)$ is understood to be $i\sqrt{V_\infty - k^2}$ for $|k| < \sqrt{V_\infty}$. We seek to compute the potential $V(x)$ for $x \geq 0$ given the reflection coefficient $R(k)$ for $k > 0$.

In general, this information is insufficient to recover V uniquely, rather one must also have available the bound state energies and corresponding norming constants. Throughout this paper we will assume that no bound states exist. This is always the case, for example, if $V(x) \geq 0$, and is generally true in the applications mentioned above.

Accounts of the classical inverse scattering problem with $V_\infty = 0$ can be found, e.g. in [3], [4], [5]. The case that $V_\infty \neq 0$ is studied in [6], [7], [8]. See also [9], [10] for some other variants. Under the assumptions we have stated, and assuming also that $V(x) - V_\infty$ decays to zero sufficiently rapidly at ∞ , then $V(x)$ for $x > 0$ is known to be uniquely determined by $R(k)$ for $k > 0$. In fact $V(x)$ is determined by either the real or imaginary part of $R(k)$ as will be discussed below. A much more interesting question in applications is whether V can be determined from $|R(k)|$ (e.g. [2]). Some partial results in this direction can be found in [11].

In principle, the potential may be computed by means of the Gelfand-Levitan-Marchenko integral equation. For $V_\infty \geq 0$ the precise procedure is the following: Set

$$g(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} R(k) e^{-ikt} dt \quad (1.4)$$

Solve the integral equation

$$K(x, t) + g(x + t) + \int_{-t}^x K(x, y) g(y + t) dy = 0 \quad x > t \quad (1.5)$$

for $K(x, t)$. Finally

$$V(x) = 2 \frac{d}{dx} K(x, x) \quad (1.6)$$

See also [6], [7], [8] for the case $V_\infty < 0$.

Examples of reconstruction based on (1.5), with $V_\infty = 0$ are given in [12]. Direct solution methods could also be based on the trace formula of [4], see e.g. [13] for examples of their use in a slightly different situation. Other methods, based on specific types of approximation of the potential are discussed in [3], [14], although the latter reference seems mostly concerned with potentials having bound states. The approach we pursue here is based on a transformation to an equivalent ‘time-domain’ problem, namely the determination of an unknown coefficient in a wave equation. One example of this kind of method may be found in [15], and in [16], [17], [18] for some related inverse spectral problems.

Another important element of our approach is the replacement of the unknown potential by an equivalent unknown ‘impedance’. The equivalence between unknown potential and

unknown impedance problems (or unknown velocity, density, index of refraction ...) is quite well known, and it is common to find the potential problem introduced as a device for studying one of these other coefficient identification problems (e.g. [12], [19]). But for computational purposes at least, we have found that there may be significant advantages to reversing this procedure. Reasons for this will be discussed further in section 4.

The outline of this paper is as follows. In section 2 we derive two time domain inverse problems equivalent to the inverse scattering problem. Section 3 contains discussion of numerical approaches for the first of these, while section 4 is concerned with the second. Finally in section 5, we state a precise algorithm for solution of the inverse scattering problem, and show some examples.

2. DERIVATION OF TIME DOMAIN PROBLEMS

Let us repeat the basic assumptions we are making concerning the potential V . We suppose that

(H) $V \in L^\infty(\mathbb{R})$, V is real valued, $V(x) \equiv 0$ for $x < 0$, $\lim_{x \rightarrow +\infty} V(x) = V_\infty \geq 0$, and V has no bound states.

We begin with a transformation to an inverse problem for a related wave equation. This part of the derivation is somewhat standard, at least for $V_\infty = 0$, (see e.g. [3], [12], [15], [20]) but we are stating it somewhat differently than is usual.

Consider a solution of

$$u_{tt} - u_{xx} + V(x)u = 0 \quad -\infty < x, t < \infty \quad (2.4)$$

corresponding to an incoming impulsive wave

$$u(x, t) = \delta(x - t) \quad t < 0 \quad (2.5)$$

We define the *impulse response function* for the potential V to be

$$g(t) = u(0, t) - \delta(t) \quad (2.6)$$

By causality we must have $u(x, t) \equiv 0$ for $x < t < -x$, $x < 0$, and so u must have the form

$$u(x, t) = g(x + t) \quad t > -x \quad x \leq 0 \quad (2.7)$$

For $x \rightarrow +\infty$, $u(x, t)$ is asymptotic to a solution $u_0(x, t)$ of

$$u_{0tt} - u_{0xx} + V_\infty u_0 = 0 \quad u_0(x, t) \equiv 0 \quad x < t \quad (2.8)$$

which always has a representation

$$u_0(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \nu(k) e^{i(\theta(k)x - kt)} dk \quad (2.9)$$

for some $\nu(k)$. Thus if

$$\hat{u}(x, k) = \int_{-\infty}^{\infty} u(x, t) e^{ikt} dt \quad (2.10)$$

and

$$\hat{g}(k) = \int_{-\infty}^{\infty} g(t) e^{ikt} dt \quad (2.11)$$

then

$$\begin{aligned} \hat{u}(x, k) &= e^{ikx} + \hat{g}(k) e^{-ikx} \quad x < 0 \\ &\sim \nu(k) e^{i\theta(k)x} \quad x \rightarrow +\infty \end{aligned} \quad (2.12)$$

It follows that $\hat{u}(x, k) = \psi(x, k)$, $R(k) = \hat{g}(k)$ and $T(k) = \nu(k)$. In particular, by the Fourier inversion theorem we have

$$g(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} R(k) e^{-ikt} dk \quad (2.13)$$

Next considerations from geometrical optics imply that

$$\lim_{t \downarrow x} u(x, t) = -\frac{1}{2} \int_0^x V(s) ds \quad (2.14)$$

Indeed if we make the expansion $u(x, t) = \delta(t - x) + A(x)H(t - x) + S(x, t)$ where H is the Heaviside function and S is continuous, then substitution into equation (2.4) and matching terms of equal singularity yields $2A'(x) + V(x) = 0$. Continuity arguments may be used to establish that $A(0) = 0$ from which (2.14) follows.

The wavefield u may thus be regarded as a solution of the following problem:

$$u_{tt} - u_{xx} + V(x)u = 0 \quad 0 < x < t < \infty \quad (2.15)$$

$$u_x(0, t) - u_t(0, t) = 0 \quad t > 0 \quad (2.16)$$

$$u(x, x) = -\frac{1}{2} \int_0^x V(s) ds \quad x > 0 \quad (2.17)$$

$$u(0, t) = g(t) \quad t > 0 \quad (2.18)$$

This is an *overdetermined* boundary value problem for u , because the equation (2.15) along with any two of the three conditions (2.16)–(2.18) determines u uniquely. In general the three boundary conditions are inconsistent, except if $V(x)$ is the exact potential. The inverse scattering problem is therefore equivalent to the following time domain coefficient determination inverse problem:

Problem I. *Determine $V(x)$ such that there exists a solution $u = u(x, t)$ of (2.15)–(2.18).*

It is known that the solution V is unique, if it exists, see further discussion below.

The second part of the transformation amounts to a change from the potential variable to an impedance variable. Denote by $a = a(x)$ the solution of

$$\sqrt{a}'' - V(x)\sqrt{a} = 0 \quad a(0) = 1 \quad a'(0) = 0 \quad (2.19)$$

We call $a(x)$ the *normalized impedance* corresponding to the potential V . The condition that V have no bound states implies that $a(x)$ exists and is positive for $x > 0$, by the Sturm comparison theorem ([21]).

Next, if $u = u(x, t)$ denotes the solution of (2.15) - (2.18) above, and

$$v(x, t) = \frac{1 + \int_x^t u(x, s) ds}{\sqrt{a(x)}} \quad (2.20)$$

then one can compute that v satisfies

$$av_{tt} - (av_x)_x = 0 \quad 0 < x < t < \infty \quad (2.21)$$

$$v_x(0, t) - v_t(0, t) = 0 \quad t > 0 \quad (2.22)$$

$$v(x, x) = \frac{1}{\sqrt{a(x)}} \quad x > 0 \quad (2.23)$$

$$v(0, t) = G(t) = 1 + \int_0^t g(s) ds \quad t > 0 \quad (2.24)$$

Again, this is an overdetermined boundary value problem for the wavefield v , and we may attempt to recover the potential V by solving:

Problem II. *Determine $a(x)$ such that there exists a solution $v = v(x, t)$ of (2.21)–(2.24).*

Then

$$V(x) = \frac{\sqrt{a(x)}''}{\sqrt{a(x)}}$$

3. COMPUTATION OF THE POTENTIAL

The occurrence of the wave equation (2.4) in connection with the inverse scattering problem is well known, but in general it has not been much exploited. Most often one sees it used in an alternative derivation of the Gelfand-Levitan-Marchenko integral equation, e.g. [3],[12],[22]. By contrast, we are suggesting that very efficient computational methods for the inverse scattering problem may be obtained by working directly with the time domain problems I and II above, avoiding any need to directly solve the Gelfand-Levitan-Marchenko equation.

There are several possibilities, which we can roughly divide into two categories, (i) iterative methods and (ii) layer stripping methods. In many situations these different techniques are quite comparable in terms of speed and accuracy. But for certain ‘large’ potentials arising in the neutron reflectivity application ([1]), we will eventually argue that the best choice is the layer stripping method applied to problem II.

Iterative methods for problem I. Problem I may be construed as a fixed point problem as follows. For a given $V \in \mathcal{A}$, define the wavefield $u = u(x, t; V)$ as the solution of the ‘sideways’ Cauchy problem

$$u_{tt} - u_{xx} + V(x)u = 0 \quad 0 < x < t < \infty \quad (3.1)$$

$$u_x(0, t) - u_t(0, t) = 0 \quad t > 0 \quad (3.2)$$

$$u(0, t) = g(t) \quad t > 0 \quad (3.3)$$

the conditions (3.1),(3.2), (3.3) determine u uniquely in the set $\{(x, t) : t > x > 0\}$, and by the same token, if g is given on the interval $[0, T]$, the field u is determined for $0 < x < t < T - x, 0 < t < \frac{T}{2}$. If we set

$$\Phi(V)(x) = -\frac{1}{2} \frac{d}{dx} u(x, x; V) \quad (3.4)$$

(where $u(x, x; V) = \lim_{t \downarrow x} u(x, t; V)$) then

$$\Phi(V) = V \quad (3.5)$$

holds if V is the correct solution. Thus we may hope that fixed point iteration

$$V_{n+1} = \Phi(V_n) \quad V_0 \equiv 0 \quad (3.6)$$

gives a sequence $\{V_n\}$ converging to the exact potential. Essentially the same mapping Φ arises in connection with some inverse spectral problems, except there the data function $g(t)$ arises in a rather different way. A proof that Φ has a unique fixed point which is the limit of the sequence V_n is given (aside from some small technicalities) in [16], Theorems 1 and 2.

Another iteration method for problem I can be derived as follows. For a given $V \in \mathcal{A}$, define the wavefield $w = w(x, t; V)$ as the solution of the Goursat problem

$$w_{tt} - w_{xx} + V(x)w = 0 \quad 0 < x < t < \infty \quad (3.7)$$

$$w_x(0, t) - w_t(0, t) = 0 \quad t > 0 \quad (3.8)$$

$$w(x, x) = -\frac{1}{2} \int_0^x V(s) ds \quad x > 0 \quad (3.9)$$

If V is given on an interval $0 < x < T/2$, the wavefield w is uniquely determined for $x < t < T - x$, $0 < x < T/2$. If we now set

$$F(V)(t) = w(0, t; V) \quad (3.10)$$

then

$$F(V) = g \quad (3.11)$$

holds if V is the correct solution. A general iterative approach to solving the functional equation (3.11) is Newton's method:

$$V_{n+1} = V_n - DF(V_n)^{-1}(F(V_n) - g) \quad (3.12)$$

with $V_0 \equiv 0$, say, and where $DF(V)$ denotes the linearization (Fréchet derivative) of F at V . The inverse operator $DF(V_n)$ may be too complicated to compute with, so we use instead the approximation $DF(V_n) \approx DF(0)$, leading to the Newton-Kantorovich (or simplified Newton) algorithm

$$V_{n+1} = V_n + DF(0)^{-1}(F(V_n) - g) \quad (3.13)$$

Calculation of $DF(0)$ is straightforward, namely

$$DF(0)\zeta(t) = -\frac{1}{2} \int_0^{\frac{t}{2}} \zeta(s) ds \quad (3.14)$$

We thus obtain that (3.13) is equivalent to

$$V_{n+1}(x) = V_n(x) + 4 \frac{d}{dt} (F(V_n) - g)|_{t=2x} \quad (3.15)$$

Although stated in somewhat different terms, the iteration method (3.15) is equivalent to the procedure derived in section 2 of [15], assuming that $V_\infty = 0$. It is also very closely related to the iteration method used in [18] to solve an inverse spectral problem, and a proof of convergence for (3.15) could be given by modification of the proof of Theorem 2.1 in [18].

Discussion of iterative methods for problem I. Either of the methods (3.6) or (3.15) is stable, fast and accurate as long as the potential V is not too large. In either case, each step of the iteration process requires that one boundary value problem for the wave equation (2.4) be solved numerically. This may be done by standard finite difference methods, with the operation count being $O(N^2)$, where N is the number of grid points at which $V(x)$ is to be recovered. Either method also requires of course that $g(t)$ be used, and we may obtain $g(t)$ from the given data $R(k)$ with the Fast Fourier Transform.

It is important to be clear about what constitutes a ‘large’ potential, because the value of $V(x)$ depends on the length units chosen. Indeed, if we perform the change of variable $x \mapsto z = x/L$, then $k \mapsto Lk$ and $V(x) \mapsto L^2V(Lz)$ in (2.2). If we think of L as a length interval of interest, and the integral average $M = \frac{1}{L} \int_0^L V(x) dx$ as a measure of the size of the potential in the given units, then the dimensionless quantity $Q = ML^2$ is invariant under rescaling of the length variable. We may therefore expect that the conditioning of the reconstruction problem is intrinsically dependent on the value of Q only. More precisely, it can be shown that there is a constant $C = C(Q_0)$, such that

$$\|V_1 - V_2\|_{H^{-1}(0,L)} \leq C(Q_0) \|g_1 - g_2\|_{L^2(0,2T)} \leq C(Q_0) \|R_1 - R_2\|_{L^2} \quad (3.15)$$

holds, if V_1, V_2 are two potentials with Q values less than Q_0 , and R_1, R_2, g_1, g_2 are the corresponding reflection coefficients and impulse response functions. Thus the effect of error in the data on the reconstructed potential is dependent on the value of Q , with the problem therefore becoming more and more ill posed as either M or L tends to infinity. It follows, at least heuristically, from estimates in Bube [23], that C is at most exponentially growing in Q , and furthermore no better result can be expected.

This kind of instability will be reflected in the failure of convergence for the iterative methods just discussed, if either M or L is too large. This is noted in [15] (p 325) and

our own experience confirms this. The neutron reflection application mentioned in the introduction leads to Q values on the order of 40 or larger, but all approaches we have tried based on problem I, even with highly accurate synthetic data, have succeeded only in the range of Q values up to 15-20. It is for this reason that we were motivated to attempt a reconstruction via the problem II instead.

4. COMPUTATION OF THE IMPEDANCE

It is not immediately apparent why there should be any significant advantage to basing computational methods on problem II, since it is just a reparameterization of problem I. The constant $C(Q_0)$ above is intrinsic, and cannot be affected by the choice of methods—there is nothing which can be done about error in the data. Nevertheless, the possibility remains that error due to discretization may be rather less in problem II than in problem I. We have found this to be the case as will be explained below, and here are some reasons for this. We are particularly indebted to K. Bube for the following discussion.

First, natural discretization methods for either the direct problem ($a \mapsto G$) or the inverse problem ($G \mapsto a$) have some unusually favorable features. Mainly they are exact, for so-called Goupillaud layered media, which is to say impedances $a(x)$ which are piecewise constant on intervals of equal length. In our case, an impedance a is continuously differentiable, with bounded second derivatives, and so can be well approximated by such a piecewise constant function. Even if an analogous discretization could be devised for problem I, the functions $V(x)$ to be approximated will be less smooth than the corresponding impedance (cf. (2.19)), and so are less accurately represented by piecewise constant functions. Put another way, the same mesh size will produce much higher accuracy for impedance than for the potential. Note also that the data function G in problem II will be more accurately represented on a grid of fixed mesh than the corresponding data $g = G'$ in problem I.

Furthermore, it is a well known and easily understood phenomena for inverse problems of this type, that errors in the reconstruction at a given depth contaminate the reconstruction at greater depths. Thus discretization errors at shallower depth have a more serious effect on the reconstruction at greater depth in the potential problem than in the impedance problem.

Finally, it is also true that to finish the reconstruction, one must differentiate the impedance twice, which is a relatively unstable procedure. However this is done *only after* the impedance has been recovered at all depths of interest. Thus the errors intro-

duced by numerical differentiation at a certain location do not have the opportunity to affect the computation of $V(x)$ at other locations. Thus, one significant source of error has been isolated, so that it cannot propagate.

Iterative methods for problem II. One can develop iteration methods for problem II, which are parallel to those mentioned above for problem I. For example, if we define the wavefield $v = v(x, t; a)$ as the solution of

$$a(x)v_{tt} - (a(x)v_x)_x = 0 \quad 0 < x < t < \infty \quad (4.1)$$

$$v_t(0, t) - v_x(0, t) = 0 \quad t > 0 \quad (4.2)$$

$$v(0, t) = G(t) \quad t > 0 \quad (4.3)$$

then v is uniquely determined, and we can set

$$\Phi(a)(x) = \frac{1}{v^2(x, x; a)} \quad (4.4)$$

The exact impedance a is thus a fixed point of Φ , and we can hope to find the solution by fixed point iteration

$$a_{n+1} = \Phi(a_n) \quad a_0(x) \equiv 1 \quad (4.5)$$

A convergence theorem for a slight modification of (4.5) is given in [17].

Layer stripping techniques. The so-called layer-stripping, or downward continuation techniques for Problem II have been introduced and studied by Bube [23], [24], Bube and Burridge[25], Santosa and Schwetlick [26], Driessel and Symes [27] and others. The idea of the method is as follows. The given data G , together with the normalization $a(0) = 1$ allows one to approximately compute the wavefield v in a shallow layer $\{(x, t) : 0 \leq x \leq \Delta x\}$ near the surface $x = 0$. The condition 2.23 is then used to obtain the value of $a(\Delta x)$. We can now repeat the procedure, obtaining $v(x, t)$ for $\Delta x < x < 2\Delta x$ and subsequently the value of $a(2\Delta x)$ from 2.23 again. Continuing in this way we obtain a piecewise constant approximation to $a(x)$ on any fixed depth interval.

For specific implementations, and error analysis as $\Delta x \rightarrow 0$, see the literature cited above. The main disadvantage, in comparison with the iterative method of the last section, is that the existing theorems require more smoothness to guarantee convergence for the layer-stripping algorithms. In practice, there seems to be no difference however, and the layer stripping method is faster, since the operation count is comparable to one iteration of (4.5).

The Fourier transformation step. Before describing the inversion algorithm we used in detail, let us first discuss the problem of accurately computing the data function $G(t)$. It is obtained by a simple quadrature from $g(t)$ which, by (2.13), is the inverse Fourier transform of the reflection data $R(k)$. One can of course use a standard FFT routine, but some less obvious methods may have some advantages from the point of view of optimal accuracy. We observe that if $R(k) = \alpha(k) + i\beta(k)$, then the fact that g must be real valued implies

$$g(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} (\alpha(k) \cos kt + \beta(k) \sin kt) dk \quad (4.6)$$

Since $g(t) = 0$ for any $t < 0$ we must also have

$$\int_{-\infty}^{\infty} \alpha(k) \cos kt dk = \int_{-\infty}^{\infty} \beta(k) \sin kt dk \quad t \geq 0 \quad (4.7)$$

(this is equivalent to the Kramers-Kronig relationship for α, β). The symmetry property $R(k) = \bar{R}(-k)$ means that α is even and β is odd, hence

$$g(t) = \frac{2}{\pi} \int_0^{\infty} \alpha(k) \cos kt dk = \frac{2}{\pi} \int_0^{\infty} \beta(k) \sin kt dk \quad (4.8)$$

i.e. g is also equal to the cosine transform of α or the sine transform of β . Computing $g(t)$ by a standard FFT amounts to averaging the two expressions in (4.8). On the other hand, there may be definite reasons for preferring one formula to the other, depending on the situation.

First of all, the impulse response always satisfies $g(0) = 0$. This is automatically true for any function computed as a sine transform, but its validity in the cosine transform representation is limited by the accuracy of the data, and its availability for large k . Thus we may expect that the second formula tends to be more accurate for small t 's. If the potential $V(x)$ to be computed has a discontinuity at $x = 0$, we have always observed considerably more 'ringing' (i.e. numerical oscillation) when the cosine transform is used.

Second, it may be the case that either α or β decays faster than the other, in which case there will be less error due to band-limitation if we choose the integral representation with the more rapidly decaying component. For example if $V(x)$ is a positive constant V_0 for $x > 0$, then $\beta(k) \equiv 0$ for $k > \sqrt{V_0}$. More generally, if V has a discontinuity at $x = 0$ and is otherwise continuously differentiable, with reasonable behavior at ∞ , then one has the asymptotic behavior

$$R(k) \sim \frac{V(0)}{4k^2} \quad k \rightarrow \infty \quad (4.9)$$

(see e.g. [11] equation (2.10)) which implies $\beta(k)/\alpha(k) \rightarrow 0$ as $k \rightarrow \infty$. On the other hand, if $V(0) = 0$, V' has jump at $x = 0$, and V is otherwise twice continuously differentiable with reasonable behavior at ∞ , then

$$R(k) \sim \frac{iV_1}{4k^3} \quad k \rightarrow \infty \quad (4.10)$$

where $V_1 = \lim_{x \rightarrow 0^+} V'(x)$, and thus $\alpha(k)/\beta(k) \rightarrow 0$. Even without this kind of *a priori* knowledge, one can always examine the given reflection data, to determine whether either α or β is significantly more rapidly decaying than the other, and then choose the formula for $g(t)$ accordingly.

A third possible consideration is to determine whether one component or the other is more well suited to approximation by sampling. When we use the grid values of α or β in computing the integrals (4.8), we are approximating the integrand between grid points by linear interpolation, and it could happen that one or the other of α, β is somewhat better approximated in this way than the other. To illustrate the point, consider the functions α, β shown in figure 1, which come from the potential reconstructed in figure 3. Both α and β have a singularity in the derivative at $k = \sqrt{V_\infty} = \sqrt{62}$, but for larger mesh sizes Δk , the approximation to α is somewhat better than that of β because of the narrow peak which β has at this k value. When the inversion procedure below is carried out, we find that we get a better result near $x = 0$ using $\beta(k)$, for the reason given in the first point above, but a better result for larger x using $\alpha(k)$ because of its better approximation property. If the mesh size is small enough, the narrow peak in β gets resolved adequately, and the reconstruction for large x is considerably better overall using β .

In this example the accuracy was assessed by comparison with the exact solution, which is ordinarily not available. Nevertheless, one can always compare the piecewise linear approximations to α, β based on a given mesh size, with the approximation based on some other mesh size, for example cutting the mesh size in half. The degree to which the two approximations differ will generally be an indication of the degree to which the exact α or β is approximated, and so a choice of which formula in (4.8) to use could be based on this comparison.

Finally, in this regard, we mention that if $V_\infty > 0$, then α and β will always have a singularity in the derivative at $k = \sqrt{V_\infty}$, so attention should be focused on k values near this point. A better approximation will generally result if it can be arranged that $k = \sqrt{V_\infty}$ is one of the grid points.

The downward continuation step. The impedance $a(x)$ is obtained from the data $G(t)$ by an application of the layer stripping method. The particular implementation we have used is taken from Bube [24], to which we refer for the exact equations. This algorithm actually requires that we make one further transformation, in order that the wavefield have nonvanishing derivatives at $x = t = 0$. We set $w(x, t) = \int_x^t v(x, t) dt$ where v is the solution of (2.21)–(2.24), so that w satisfies

$$aw_{tt} - (aw_x)_x = 0 \quad 0 < x < t < \infty \quad (4.11)$$

$$w_t(0, t) = G(t) \quad t > 0 \quad (4.12)$$

$$w_x(0, t) = G(t) - 2 \quad t > 0 \quad (4.13)$$

$$w(x, x) = 0 \quad x > 0 \quad (4.14)$$

The condition (4.14) means that w is a *causal* solution of (4.11), so that the analysis of [24] applies. The input to the algorithm is $G(t)$ sampled at points $t = t_j = j\Delta t$, and the output is an approximation to $a(x)$ sampled at half-integer mesh points $x_i = (i + \frac{1}{2})\Delta x$, $\Delta x = \Delta t/2$. The accuracy is $O((\Delta x)^2)$.

5. ALGORITHM AND EXAMPLES

We describe now the details of a procedure for reconstructing the potential, based on applying the layer-stripping method to problem II above. The input to the algorithm consists of

- (1) An interval length L on which the potential $V(x)$ is to be found.
- (2) Sampled reflection data $R(k)$ for $k = j\Delta k, j = 1, \dots, M$.

The eventual output will be an approximate $V(x)$ sampled at points $x = i\Delta x, i = 0, \dots, N$ with $N\Delta x = L$.

Step 1. We normalize the length units so that $L = 1$ by the transformation $\Delta k \mapsto L\Delta k$.

Step 2. We obtain the data function $g(t)$ for $0 \leq t \leq 2$, sampled at points $t = i\Delta t$ with $\Delta t = \frac{2}{3N}$, using the fast sine or fast cosine transform, as indicated above. We remark that $R(0) = -1$ always holds under our assumptions. Also, the factor of 3 is present, because we will solve for the impedance on grids of mesh size $\frac{1}{3N}$ and $\frac{1}{N}$, and then use an extrapolation step.

Step 3. We obtain the data function $G(t)$ by numerical integration of the sampled $g(t)$. We remark that if one is attempting to reconstruct potentials which aren't very smooth, it is advisable *not* to use a high order quadrature rule, since this may actually be less accurate when applied to non-smooth functions. In the examples below, the trapezoid rule was used. We note also that it is possible to derive a direct Fourier representation for G , but the results were not as accurate as when we do the integration step explicitly.

Step 4. The sampled $G(t)$ is now used as input to the layer stripping algorithm as described above. As was already mentioned, we carry out this step on a fine grid, $\Delta x = \frac{1}{3N}$, and on a coarse grid, $\Delta x = \frac{1}{N}$. Since the resulting approximations to $a(x)$ are given on half integer grids, the purpose of the factor of 3 is now clear, namely this is what is needed in order that the coarse grid be a subset of the fine grid.

Step 5. We extrapolate to zero grid size. If we denote $a^h(x_i)$ the approximation to $a(x_i)$ based on grid size h , the error estimate of Bube [24] is that

$$a(x_i) = a^h(x_i) + O(h^2) \tag{5.1}$$

for sufficiently smooth impedance a . Thus the appropriate extrapolation formula is

$$a(x_i) \approx \frac{9a^h(x_i) - a^{3h}(x_i)}{8} \tag{5.2}$$

which we apply with $h = \frac{1}{3N}$ and each half integer mesh point $x_i = \frac{2i+1}{2N}$ of the coarse grid.

Step 6. We can obtain the sampled values for the potential $V(x) = \sqrt{a(x)''}/\sqrt{a(x)}$ with standard difference approximations to the second derivative. We return to the original units, $x_i \rightarrow Lx_i$ and $V(x_i) \rightarrow V(x_i/L)/L^2$. If necessary, one can interpolate to get $V(x)$ on the standard grid $x_i = i\Delta x$ instead of the half integer grid $x_i = \frac{L}{N} \frac{2i+1}{2}$.

We now show examples of potential reconstruction, using this algorithm. The first example is

$$V(x) = \frac{8}{(1+2x)^2} \tag{5.3}$$

for which the reflection is known analytically ([28]),

$$R(k) = \frac{2}{k^2 + 2ik - 2}$$

We took $L = 10$, $\Delta k = .05$, $N = 200$, and $M = 200$, and carried out the above algorithm using both the sine and the cosine transform formulas to compute $g(t)$ in step 2. The

results are shown along with the exact solution in figure 2. As expected we obtain a much better result using the sine transform, since the imaginary part of $R(k)$ decays much more rapidly than the real part (cf. 4.9). The Q value in this case is about 18.

The second example (figure 3) shows the reconstruction of the potential in figure 2, for which $Q \approx 39$, using $L = 1$, $\Delta k = .025$, $N = 200$ and $M = 4000$. The scattering data here was generated by straightforward numerical integration of (1.2), assuming that V is constant for $x > L$. Again the imaginary part decays somewhat faster than the real part, so we used the sine transform to compute $g(t)$.

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Figure Captions

Figure 1: Real and imaginary parts of $R(k) = \alpha(k) + i\beta(k)$ for the potential shown in figure 3.

Figure 2: Exact potential $V(x) = \frac{2}{(1+x)^2}$ for $x > 0$, and reconstructions from reflection data.

Figure 3: Reconstruction of potential from reflection data.