

# Multidimensional inverse scattering: An orthogonalization formulation

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The three-dimensional Schrödinger equation inverse scattering problem is solved using an orthogonalization approach. The plane waves propagating in free space are orthogonalized with respect to an inner product defined in terms of a Jost operator. The resulting integral equation is identical to the generalized Gel'fand–Levitan equation of Newton, although the present derivation is simpler and more physical than that of Newton. Newton's generalized Marchenko equation is derived from the defining integral equation for the Jost operator. These integral equations are shown to be solved by fast algorithms derived directly from the properties of their solutions. This paper thus presents a simple interpretation of Newton's two integral equations, two fast algorithms for solving these integral equations, and relations between the various approaches. This is a generalization of previously obtained results, which are also reviewed here, for the one-dimensional inverse scattering problem.

## I. INTRODUCTION

The inverse scattering problem for the Schrödinger equation in three dimensions with a time-independent, local, non-spherically-symmetric potential has a wide variety of applications. For example, the inverse seismic problem of reconstructing the density and wave speed of an inhomogeneous isotropic acoustic medium from surface measurements of the medium response to a harmonic excitation can be formulated as a Schrödinger equation inverse scattering problem, as was done by Coen *et al.*<sup>1</sup>

A major breakthrough in obtaining an *exact* solution to the three-dimensional Schrödinger equation inverse scattering problem was made by Newton.<sup>2</sup> In Ref. 2 Newton presented generalized versions of two integral equations obtained for the *one-dimensional* inverse problem by Marchenko<sup>3</sup> and Gel'fand and Levitan.<sup>4</sup> These *generalized* Marchenko and Gel'fand–Levitan integral equations reconstruct the scattered field in the vicinity of the scattering potential from far-field data, just as their one-dimensional namesakes do (for details of the one-dimensional problem integral equations, see Refs. 5 and 6). The scattering potential is then recovered from the scattered field using an equation Newton calls the “miracle” equation. This completes the solution of the inverse scattering problem. In Ref. 1 this procedure was applied to the inverse seismic problem noted above.

Recently it has been noted that the derivation of the generalized Gel'fand–Levitan integral equation in Ref. 2 relies implicitly on the existence of a so-called “regular” solution. It was not firmly established in Ref. 2 that this regular solution is always well defined. However, this does not invalidate the results of Ref. 2; it merely limits their applicability to situations for which the regular solution *does* exist. In this paper the inverse scattering problem is restricted to situations in which the regular solution exists and is well defined; this is expected to cover most physical inverse scattering problems. Since a major goal of this paper is to underscore ways in which one-dimensional results generalize to three dimensions, this is an acceptable limitation.

Although Ref. 2 is a highly significant contribution to inverse scattering theory, the derivations contained therein shed little insight into the actual mechanism of the inversion process. Several recent papers have presented much simpler derivations of Newton's Marchenko integral equation. In Ref. 7 the frequency-domain Schrödinger equation was transformed into a time-domain plasma wave equation, and the interpretation of various frequency-domain properties (e.g., analyticity in the upper half-plane) as time-domain properties (e.g., causality) lent some physical insight into the inversion process. Newton's Marchenko integral equation was derived in Ref. 8 using a representation theorem, and was derived in Ref. 9 using a generalized Radon transform; both of these derivations are much simpler than Newton's derivation. However, there are no such simpler derivations as yet for Newton's generalized Gel'fand–Levitan integral equation.

For the one-dimensional inverse problem the integral equation procedures of Refs. 3–6 are known to have *differential* counterparts, which are called *layer stripping* algorithms (in the seismic literature they are known as “downward continuation” algorithms). These algorithms may be derived by exploiting the Toeplitz or Hankel structure of the kernel of integral equations<sup>10</sup>; however, derivations that are more physical and insightful result if basic physical principles such as causality are exploited.<sup>11</sup> Since they exploit the inherent structure of the inverse scattering problem, which manifests itself in the structure of the kernel of the integral equation, these algorithms require significantly fewer computations than would solving the integral equations; hence they are referred to as “fast” algorithms. An important point is that these differential, layer stripping algorithms are intimately related to the integral equation procedures; these relations are discussed in Ref. 11.

Layer stripping algorithms for the three-dimensional Schrödinger equation inverse scattering problem have been proposed in Refs. 9 and 12. Although the numerical performance of these algorithms is unknown at present, their computational complexity is significantly less than that of the

integral equation procedures of Newton. A relation between the algorithm of Ref. 9 and Newton's Marchenko integral equation procedure was presented in Ref. 9; this relation involved a generalized Radon transform. However, this relation did not extend to Newton's generalized Gel'fand-Levitan integral equation, and a differential fast algorithm for this integral equation has not been obtained previously.

In this paper Newton's generalized Gel'fand-Levitan integral equation is rederived by treating the inverse scattering problem as an orthogonalization problem. A Gram-Schmidt orthonormalization is performed on the free-space form of the wave field, which is a probing plane wave in a given direction of incidence. The orthogonalization is performed with respect to an inner product defined in terms of a multidimensional Jost operator, and the associated orthogonality principle results in Newton's generalized Gel'fand-Levitan integral equation. This is the first derivation of this equation other than that of Ref. 2. Newton's generalized Marchenko integral equation is also derived from the integral equation defining the Jost operator.

Two differential fast algorithms that also solve these integral equations are given. One of these algorithms is the algorithm of Ref. 12; the other is a generalized Levinson-like algorithm that is new, although it bears some resemblance to a fast algorithm derived in Ref. 13 for the problem of computing the filter for the linear, least-squares estimate of a homogeneous, anisotropic random field.

This paper thus provides a unified derivation of two multidimensional integral equations and two multidimensional fast algorithms, all of which solve the inverse scattering problem for the three-dimensional Schrödinger equation. It is thus a generalization of results for the one-dimensional inverse problem presented in Refs. 11 and 14, and illustrates how all of these procedures are connected.

The paper is organized as follows. Results for one dimension are quickly summarized in Sec. II, which contains some results from Refs. 11 and 14. The new results for three dimensions are contained in Sec. III, and the ways in which the one-dimensional results generalize to three dimensions are emphasized. The main results of Sec. III are Newton's generalized Gel'fand-Levitan and Marchenko integral equations. In Sec. IV the differential, layer-stripping algorithms are presented and related to the integral equations of Sec. III. Some connections between multidimensional inverse scattering and linear, least-squares estimation of homogeneous, anisotropic random fields are also noted. Finally, Sec. V concludes by summarizing the results of the paper and noting directions in which further research is needed.

## II. THE ONE-DIMENSIONAL PROBLEM

This section derives the Gel'fand-Levitan and Marchenko integral equations for the one-dimensional inverse scattering problem using an orthogonalization procedure, following Ref. 14. It also derives differential fast algorithms that solve the inverse scattering problem and require fewer computations than would solving the integral equations. The purpose of this section is to review these concepts in a simple setting before proceeding to the more complex three-dimensional inverse problem, and to demonstrate how the

concepts for the one-dimensional case generalize to the three-dimensional case.

### A. The fundamental solutions

The one-dimensional inverse scattering problem considered in this section is as follows. The wave field  $u(x,k)$  satisfies the Schrödinger equation

$$\left(\frac{d^2}{dx^2} + k^2 - V(x)\right)u(x,k) = 0, \quad (2.1)$$

where the scattering potential  $V(x)$  is real valued, smooth, and has compact support. Two different initial conditions for this differential equation will be considered, resulting in two different solutions. These correspond to two different inverse scattering problems: the reflection problem and the regular problem. The names of these problems come from the names of their solutions, as will be explained shortly.

The time-domain version of the Schrödinger equation (2.1) is the *plasma wave equation*

$$\left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial t^2} - V(x)\right)\check{u}(x,t) = 0. \quad (2.2)$$

Solutions of (2.2) are related to solutions of (2.1) by a Fourier transform. In the sequel we will switch freely from the time domain to the frequency domain and back again.

First, some solutions to the *reflection* problem are defined. The wave field  $u(x,k)$  is split into two waves traveling in the  $+x$  and  $-x$  directions, and two different reflection problems (probing from  $-\infty$  and  $+\infty$ ) are considered. This results in four solutions, which are then arranged in a  $2 \times 2$  matrix  $\Psi(x,k)$  and termed the *Jost* solution. The components of the Jost solution  $\Psi(x,k) = [\psi(x,k,+), \psi(x,k,-)]^T$  to (2.1) are defined by their behavior at  $\pm\infty$ . Specifically,

$$\psi(x,k,+) = [e^{-ikx}, R_L(k)e^{ikx}]^T \text{ as } x \rightarrow -\infty, \quad (2.3a)$$

$$\psi(x,k,+) = [T(k)e^{-ikx}, 0]^T \text{ as } x \rightarrow \infty, \quad (2.3b)$$

$$\psi(x,k,-) = [0, T(k)e^{ikx}]^T \text{ as } x \rightarrow -\infty, \quad (2.3c)$$

$$\psi(x,k,-) = [R_R(k)e^{-ikx}, e^{ikx}]^T \text{ as } x \rightarrow \infty. \quad (2.3d)$$

Physically, the solution  $\psi(x,k,+)$  results from a problem in which the scattering potential is probed from the left, in the  $+x$  direction, resulting in a transmitted wave  $T(k)e^{-ikx}$  and a reflected wave  $R_L(k)e^{ikx}$ . The solution  $\psi(x,k,-)$  results from a problem in which probing takes place from the right, in the  $-x$  direction. Here  $R_L(k)$  and  $R_R(k)$  are the *reflection coefficients* for the two problems, and  $T(k)$  is the *transmission coefficient*, which by reciprocity is the same for both problems. The first component of each solution is the rightward traveling wave, and the second component is the leftward traveling wave. The situation is illustrated in Fig. 1. Note that the complete Jost solution  $\Psi(x,k)$  is thus a  $2 \times 2$  matrix. Since the data for these problems consists of the reflection coefficient  $R_L(k)$  or  $R_R(k)$ , the inverse scattering problem that results in the Jost solution  $\Psi(x,k)$  is termed the *reflection problem*. Note that given either  $R_L(k)$  or  $R_R(k)$  it is possible to reconstruct the other reflection coefficient and  $T(k)$ ; see Ref. 6.

Next, some solutions to the *regular* problem are defined. The wave field  $u(x,k)$  is again split into two waves traveling

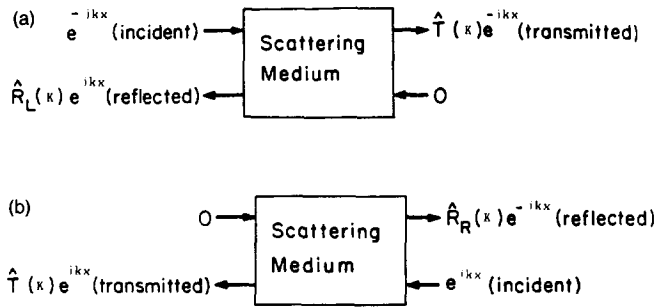


FIG. 1. (a) The reflection problem for an impulsive plane wave incident from the left. (b) The reflection problem for an impulsive plane wave incident from the right.

in the  $+x$  and  $-x$  directions; however, the boundary conditions are changed. Instead of specifying the behavior of the wave field at  $\pm\infty$ , the behavior is specified at the origin  $x=0$ . Since each wave must be initialized, this again results in a  $2 \times 2$  matrix. The *regular* solution  $\Phi(x,k) = [\phi(x,k,+), \phi(x,k,-)]^T$  to (2.1) is defined by the initial conditions

$$\Phi(0,k) = I_2, \quad \frac{d}{dx} \Phi(0,k) = \text{diag}[ik, -ik]. \quad (2.4)$$

In the time domain, this corresponds to introducing an impulse at the origin  $x=0$ . Thus in the time domain the regular solution is actually a noncausal impulse response relating the field at the origin to the field at  $x$ . This is discussed in more detail in Ref. 15. The term “regular solution” was introduced by Newton in Ref. 2, and has become standard; hence we use it here. The inverse scattering problem resulting in the regular solution  $\Phi(x,k)$  is termed the *regular problem*, and it is illustrated in Fig. 2.

Since the reflection and regular solutions are linearly independent, they are related by a *Jost function*  $J(k)$ , which is also a  $2 \times 2$  matrix. We have

$$\Phi(x,k) = \Psi(x,k)J(k) \quad (2.5)$$

and at  $x=0$  we also have

$$\Psi(0,k) = \Phi(0,k)J^{-1}(k) = J^{-1}(k). \quad (2.6)$$

Since the total field  $u(x,k)$  is the sum of the leftgoing and rightgoing waves at  $x$ , we have

$$u(0,k) = [1, 1]J^{-1}(k). \quad (2.7)$$

All of these equations generalize directly to the three-dimensional case, as we shall see in Sec. III.

Since the one-dimensional problem is defined on the entire real line, and the potential  $V(x)$  has compact support, we may without loss of generality restrict its support to the half-line  $x \geq 0$ . Then the Jost solution condition at  $-\infty$  may be replaced by a similar condition at  $x=0$ . Equations (2.3) and (2.6) then yield

$$J^{-1}(k) = \begin{bmatrix} 1 & 0 \\ R_L(k) & T(k) \end{bmatrix}. \quad (2.8)$$

This explicit representation of the Jost function will not be available in the three-dimensional case, since that problem is radial, i.e., defined on  $|x| \geq 0$ .

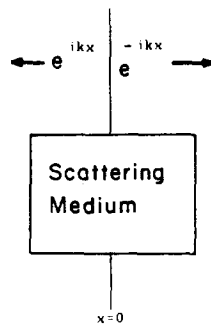


FIG. 2. The regular problem. For the 1-D problem: an impulsive boundary condition at  $x=0$ . For the 3-D problem: an impulsive boundary condition on the plane  $e_i \cdot x = 0$ .

## B. Orthogonalization

It is well known that the Jost solutions  $\Psi(x,k)$  are orthonormal on the real line with respect to the usual  $L^2$  matrix inner product, i.e., that

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \Psi(x,k) \Psi(y,k)^H dk = \delta(x-y), \quad (2.9)$$

where the superscript H denotes Hermitian transpose. This naturally suggests that the reconstruction of the field resulting from a scattering problem might be regarded as an orthogonalization procedure. However, such a procedure would clearly have to start from a point and proceed outward, and for the Jost solutions there is no clear place to start. The regular solutions  $\Phi(x,k)$  would be an ideal candidate for such a procedure, since they are formed starting at  $x=0$  and propagate outward in the  $\pm x$  directions, but they are not orthonormal. But the regular solutions *are* orthonormal with respect to the inner product with weighting matrix  $(J^H J)^{-1}(k)$ , since

$$\begin{aligned} \frac{1}{2\pi} \int_{-\infty}^{\infty} \Phi(x,k) (J^H J)^{-1}(k) \Phi(y,k)^H dk \\ = \frac{1}{2\pi} \int_{-\infty}^{\infty} \Psi(x,k) \Psi(y,k)^H dk = \delta(x-y). \end{aligned} \quad (2.10)$$

Note that

$$(J^H J)^{-1}(k) = \begin{bmatrix} 1 & R_L^*(k) \\ R_L(k) & 1 \end{bmatrix}, \quad (2.11)$$

which follows from (2.8) and the conservation of energy relation

$$|R_L(k)|^2 + |T(k)|^2 = 1. \quad (2.12)$$

This suggests that the solutions  $\Phi(x,k)$  may be constructed from the scattering data from the left,  $R_L(k)$ , as follows.

The quantities to be orthogonalized are, in the time domain, the free-space leftgoing and rightgoing impulsive plane waves resulting from the impulse introduced at the origin. In the frequency domain, these waves have the form  $e^{\pm ikx}$ , and arranging them into a  $2 \times 2$  matrix as was done with the reflection and regular solutions results in the *free-space* solutions

$$E(x,k) = \begin{bmatrix} e^{-ikx} & 0 \\ 0 & e^{ikx} \end{bmatrix}. \quad (2.13)$$

In the absence of a scattering potential these would constitute the regular solution to the Schrödinger equation (2.1), so that we *would* have  $\Phi(x,k) = E(x,k)$ .

Since there is a scattering potential, the solution  $\Phi(x,k)$  is formed by *orthogonalizing*  $E(x,k)$  in increasing  $|x|$ . This is done by projecting  $E(x,k)$  onto the subspace of already-orthogonalized  $\Phi(x,k)$ , which is  $\text{span}\{\Phi(y,k), |y| < |x|\} = \text{span}\{E(y,k), |y| < |x|\}$ . The projection onto a subspace is a linear combination of the elements of the subspace; here it takes the form

$$\mathcal{P}\{E(x,k)\} = - \int_{-x}^x M(x,y)E(y,k)dy, \quad (2.14)$$

where  $M(x,y)$  is a matrix kernel to be specified momentarily. Note that the linear combination has been taken over the elements of  $\text{span}\{E(y,k), |y| < |x|\}$ , rather than  $\text{span}\{\Phi(y,k), |y| < |x|\}$ ; since the orthogonalization of a subspace does not change its span these two subspaces are equal, and the projection can be taken to be a linear combination of the elements of either subspace.

The error  $E(x,k) - \mathcal{P}\{E(x,k)\}$  is then orthogonal to the above subspace, and we take the error to be  $\Phi(x,k)$ . We now recognize  $M(x,t)$  to be the *smooth* part of the inverse Fourier transform of  $\Phi(x,k)$ ,

$$\Phi(x,k) = \text{diag}[e^{-ikx}, e^{ikx}] + \int_{-x}^x M(x,t)e^{-ikt} dt, \quad (2.15)$$

so that  $M(x,t)$  is the *scattered* part of the regular solution to the plasma wave equation (2.2), which is the Schrödinger equation in the time domain.

Writing out the condition that the error  $\Phi(x,k)$  be orthogonal to  $E(y,k)$  with respect to the inner product defined in (2.9) for  $|y| < |x|$  results in the following integral equation for the scattered field  $M(x,t)$ :

$$\begin{bmatrix} 0 & R(x+t) \\ R(x+t) & 0 \end{bmatrix} + M(x,t) + \int_{-t}^x M(x,y) \begin{bmatrix} 0 & R(y+t) \\ R(y+t) & 0 \end{bmatrix} dy = 0, \quad (2.16)$$

where

$$R(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} R_L(k)e^{ikt} dk \quad (2.17)$$

is the inverse Fourier transform of  $R_L(k)$ . Note that  $R(t)$  is a *causal* function, which accounts for the lower limit of the integral in (2.16). The centrosymmetry of (2.16) implies that  $M(x,t)$  is a centrosymmetric matrix, i.e., that

$$M_{11}(x,t) = M_{22}(x,t), \quad M_{12}(x,t) = M_{21}(x,t) \quad (2.18)$$

[note that this also follows on purely physical grounds from the definition of  $\Phi(x,k)$ ]. This implies that the *scattered field*  $\check{u}_s(x,t)$ , which is the sum of the waves traveling in the  $\pm x$  directions, i.e.,

$$\check{u}_s(x,t) = M_{11}(x,t) + M_{21}(x,t), \quad (2.19)$$

satisfies the *Gel'fand-Levitan integral equation*

$$R(x+t) + \check{u}_s(x,t) + \int_{-t}^x \check{u}_s(x,y)R(y+t)dy, \quad -x \leq t \leq x. \quad (2.20)$$

Equation (2.20) is a Gel'fand-Levitan equation since the unknown scattered field  $\check{u}_s(x,t)$  arising from a *regular*

problem has finite support  $-x \leq t \leq x$ , resulting in a finite interval of integration.

The *Marchenko* equation for this problem has the same form, except that the range of validity is changed to  $t \geq x$ . This follows since it has been assumed that the potential  $V(x)$  has support on the half-line  $x \geq 0$ . Thus there is no difference between the regular and reflection *problems*, so that the only difference between the regular and reflection (*Jost*) *solutions* is their supports, which are complementary.

The half-line assumption was necessary in order to obtain an explicit representation of the inverse Jost function  $J^{-1}(k)$ . In the three-dimensional case an explicit representation of  $J^{-1}(k)$  will not be available, and the distinction between the two integral equations will become important. This distinction is also important in the one-dimensional inverse problem on the *full (real) line*.

For both the regular and Jost solutions, the potential  $V(x)$  may be obtained from the jump in the scattered field at the wave front, as follows. The solution to the plasma wave equation (2.2) can be written as

$$\check{u}(x,t) = \delta(t-x) + \check{u}_s(x,t)1(t-x) \quad (2.21a)$$

for the reflection problem, and

$$\check{u}(x,t) = \delta(t-x) + \check{u}_s(x,t)(1(t+x) - 1(t-x)) \quad (2.21b)$$

for the regular problem, where  $\check{u}_s(x,t)$  is the smooth part of the scattered field and  $1(\cdot)$  is the unit step or Heaviside function. Inserting (2.21) in (2.2) and equating orders of singularities yields<sup>16</sup>

$$V(x) = \pm 2 \frac{d}{dx} \check{u}_s(x,x), \quad (2.22)$$

where the  $+$  applies for the regular problem and the  $-$  for the reflection problem. Equation (2.22) in conjunction with the integral equation (2.20) completes the solution of the inverse scattering problem.

### C. Fast algorithms

An alternative to solving the integral equation (2.20) is to propagate the scattered field  $\check{u}_s(x,t)$  for all  $t$  recursively in  $x$ , obtaining  $V(x)$  from (2.22) as we go. This is the essence of a *layer stripping* algorithm, which recursively reconstructs the scattered field and potential and strips away their effects. However, the layer stripping algorithms for the regular and reflection problems, although superficially similar in appearance, are actually quite different. The difference is due to the complementary nature of the support of the scattered fields for the two problems, as illustrated in Figs. 3 and 4. The regular solution in the time domain, which is  $\text{diag}[\delta(t-x), \delta(t+x)] + M(x,t)$ , has support in  $t$  in the interval  $[-x, x]$ . The reflection solution in the time domain has support in  $t$  in the interval  $[x, \infty]$  for the problem in which probing takes place from the left, and has support in  $t$  in the interval  $[-\infty, -x]$  for probing from the right. This produces a major difference in the manner in which (2.22) is implemented in the algorithms.

A fast algorithm that recursively reconstructs the potential and scattered field for the *reflection* problem is as follows.<sup>11</sup>

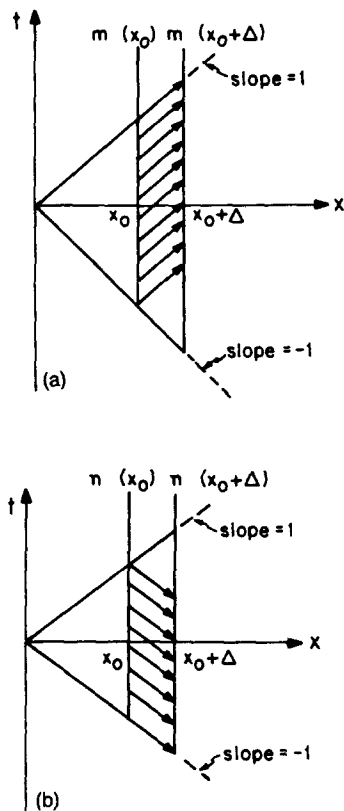


FIG. 3. (a) Recursion pattern for updating  $m(x,t)$  in the fast algorithm for the regular problem. (b) Recursion pattern for updating  $n(x,t)$  in the fast algorithm for the regular problem.

(1) Initialize the algorithm with

$$\ddot{u}(0,t) = R(t), \quad \check{q}(0,t) = 2 \frac{d}{dt} R(t). \quad (2.23)$$

(2) Propagate the following equations recursively in  $x$  and  $t$ , for  $t > x$ :

$$\left( \frac{\partial}{\partial x} + \frac{\partial}{\partial t} \right) \ddot{u}(x,t) = \check{q}(x,t), \quad (2.24a)$$

$$\left( \frac{\partial}{\partial x} - \frac{\partial}{\partial t} \right) \check{q}(x,t) = V(x) \ddot{u}(x,t), \quad (2.24b)$$

$$V(x) = -2\check{q}(x,x). \quad (2.24c)$$

The recursion pattern for this algorithm is illustrated in Fig. 4. Note that this amounts to successively truncating the potential—at each recursion, the region to the left of  $x$  has been replaced by free space [ $V(y) = 0$  for  $y < x$ ]. Thus the algorithm is successively reconstructing the potential and then stripping away its effects; hence the name “layer stripping” algorithm.

A fast algorithm that recursively reconstructs the potential and scattered field for the *regular* problem is as follows. For convenience let the *scalars*  $m(x,t)$  and  $n(x,t)$  constitute the first column of the *matrix*  $M(x,t)$  of (2.14), i.e.,  $m(x,t) = M_{11}(x,t)$  and  $n(x,t) = M_{21}(x,t)$ . Then proceed as follows.

(1) Initialize the algorithm with

$$m(0,t) = n(0,t) = 0. \quad (2.25)$$

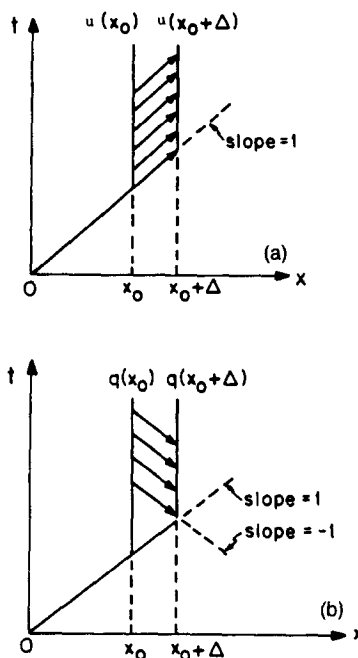


FIG. 4. (a) Recursion pattern for updating  $u(x,t)$  in the fast algorithm for the reflection problem. (b) Recursion pattern for updating  $q(x,t)$  in the fast algorithm for the reflection problem.

(2) Propagate the following equations recursively in  $x$  and  $t$ , for  $-x < t < x$ :

$$\left( \frac{\partial}{\partial x} + \frac{\partial}{\partial t} \right) m(x,t) = n(x,t), \quad (2.26a)$$

$$\left( \frac{\partial}{\partial x} - \frac{\partial}{\partial t} \right) n(x,t) = V(x) m(x,t), \quad (2.26b)$$

$$m(x,t = -x) = 0, \quad (2.26c)$$

$$\begin{aligned} V(x) &= 2n(x,x) \\ &= -4 \frac{d}{dt} R(2x) - 2R(2x)m(x,x) \\ &\quad + \int_{-x}^x m(x,y) \frac{d}{dt} R(x+y) dy \\ &\quad + \int_{-x}^x R(x+y) \left\{ n(x,y) - \frac{d}{dt} R(x+y) \right. \\ &\quad \left. - \int_{-y}^x m(x,z) \frac{d}{dy} R(z+y) dz \right\} dy, \end{aligned} \quad (2.26d)$$

where (2.26d) follows from applying (2.26a) to the integral equation (2.20).

The recursion pattern for this algorithm is illustrated in Fig. 3. Note that for the regular problem the support in  $t$  of  $m(x,t)$  and  $n(x,t)$  is the interval  $[-x, x]$ , so that the data  $R(t)$  enters into the algorithm not in the initialization, but in the computation of  $V(x)$  at each recursion. Thus this algorithm solves a *boundary value* problem, while the reflection problem algorithm solves an *initial value* problem. This is why the additional computation of (2.26d) is necessary for the regular problem algorithm, but not for the reflection problem algorithm.

Let the region where  $V(x)$  has support be discretized

into  $N$  subintervals. Then each of these algorithms requires  $O(N)$  multiplication-and-add operations at each recursion, for a total of  $O(N^2)$  operations to reconstruct  $V(x)$ . Solution of the integral equations by Gaussian elimination requires  $O(N^3)$  operations to reconstruct  $V(x)$ . The fast algorithms require fewer computations because they exploit the causal structure of the inverse scattering problem. Both of these algorithms have their three-dimensional problem counterparts, which are given in Sec. IV.

It should be noted that other differential fast algorithms exist; see Ref. 11. In particular, the more familiar continuous-parameter fast Cholesky and Krein–Levinson algorithms can be derived by reformulating the Schrödinger equation as a two-component wave system parametrized by a reflectivity function. Details are given in Ref. 11.

In this section the Gel'fand–Levitan integral equation has been derived by considering the inverse scattering problem as an orthogonalization problem with respect to the inner product defined in (2.10). This result has appeared previously in Refs. 14 and 17; it has been reviewed here in order to make apparent the ways in which this approach generalizes to the three-dimensional problem. In the next section the three-dimensional problem is treated using a similar approach, and generalized Gel'fand–Levitan and Marchenko integral equations identical to those of Ref. 2 are obtained.

### III. THE THREE-DIMENSIONAL PROBLEM

In this section the main results of this paper are presented. The generalized Gel'fand–Levitan and Marchenko integral equations derived in Ref. 2 are here derived using an orthogonalization procedure similar to that used above for the one-dimensional problem. This is a much simpler derivation than the one used in Ref. 2, and it clarifies the difference between the solutions of the two integral equations. It also illustrates how the one-dimensional results presented above generalize to three dimensions.

#### A. The fundamental solutions

The inverse scattering problem considered in this section is as follows. The wave field  $u(\mathbf{x}, k)$  satisfies the Schrödinger equation

$$(\Delta + k^2 - V(\mathbf{x}))u(\mathbf{x}, k) = 0, \quad (3.1)$$

where  $\mathbf{x} \in \mathbb{R}^3$  and the potential  $V(\mathbf{x})$  is real valued, smooth, and has compact support. It is also assumed that  $V(\mathbf{x})$  does not induce bound states; a sufficient condition for this is for  $V(\mathbf{x})$  to be non-negative. It should be noted that bound states are treated in Ref. 2; we omit them in the present derivation for simplicity and to emphasize the parallels with the one-dimensional problem. The time-domain version of (3.1) is again the plasma wave equation<sup>7,8</sup>

$$\left(\Delta - \frac{\partial^2}{\partial t^2} - V(\mathbf{x})\right)\tilde{u}(\mathbf{x}, t) = 0, \quad (3.2)$$

where solutions to (3.1) and (3.2) are related by a Fourier transform. As before, we will switch freely from the time domain to the frequency domain, and back again.

As in the one-dimensional problem, two different sets of boundary conditions are specified, resulting in two different

solutions. To emphasize the parallels with the one-dimensional problem, we use the same notation as in Sec. II.

Let  $\psi(\mathbf{x}, k, \mathbf{e}_i)$  be the solution to (3.1) with boundary condition

$$\psi(\mathbf{x}, k, \mathbf{e}_i) = e^{-ike_i \cdot \mathbf{x}} + (e^{-ik|\mathbf{x}|}/4\pi|\mathbf{x}|)A(k, \mathbf{e}_s, \mathbf{e}_i) + O(|\mathbf{x}|^{-2}), \quad (3.3)$$

where the scattering amplitude is defined by

$$A(k, \mathbf{e}_s, \mathbf{e}_i) = - \int e^{-ike_i \cdot \mathbf{y}} V(\mathbf{y}) \psi(\mathbf{y}, k, \mathbf{e}_i) d\mathbf{y} \quad (3.4)$$

and  $\mathbf{e}_i$  and  $\mathbf{e}_s$  are unit vectors. The solutions  $\psi(\mathbf{x}, k, \mathbf{e}_i)$  can be considered as a generalization of the one-dimensional Jost solutions (as in Ref. 2), with the ensemble of directions  $\{\mathbf{e}_i\}$  replacing the directions  $\pm x$ . These solutions also result from a reflection problem in which an incident impulsive plane wave in the direction  $\mathbf{e}_i$  is used to probe the scattering potential, and the data consists of the far-field reflection response in the form of the scattering amplitude. Equations (3.3) and (3.4) have their time-domain counterparts that specify solutions to the plasma wave equation (3.2); see Refs. 7–9. Note that in the present formulation the factor of  $4\pi$  is incorporated in (3.3) instead of (3.4), as in Refs. 7–9.

Let  $\phi(\mathbf{x}, k, \mathbf{e}_i)$  be the solution to (3.2) that is an entire analytic function of  $k$ , is of exponential order  $|\mathbf{e}_i \cdot \mathbf{x}|$ , and has a value of 1 along the plane  $\mathbf{e}_i \cdot \mathbf{x} = 0$ . More specifically,  $\phi(\mathbf{x}, k, \mathbf{e}_i)$  is specified by the boundary conditions

$$\phi(\mathbf{x}, k, \mathbf{e}_i) = 1; \quad \nabla \phi(\mathbf{x}, k, \mathbf{e}_i) = ike_i \quad \text{for } \mathbf{e}_i \cdot \mathbf{x} = 0; \quad (3.5)$$

$\phi(\mathbf{x}, k, \mathbf{e}_i)$  is thus a generalization of the regular solution (2.4) to three dimensions. It is also the regular solution referred to in Ref. 2.

In Ref. 17 it was pointed out that the regular solution defined in Ref. 2 cannot be guaranteed to exist. This is because the regular solution in Ref. 2 was *defined* by a Jost operator [Eq. (3.6) below; compare to (2.5) for the one-dimensional problem], and thus it cannot be guaranteed to be of exponential order  $|\mathbf{e}_i \cdot \mathbf{x}|$ . This implies that the Povsner–Levitan relation (7.3) used in Ref. 2 may be incorrect. Here, however, we *assume* that this regular solution exists.

It should be noted that the existence of the regular solution in general is still an unsolved problem. However, the corrections made to the results of Ref. 2 in Refs. 18 and 19 obfuscate an already complicated inverse scattering procedure still further, and as noted in Ref. 18, the results of Ref. 2 are “probably correct” in any case. In the sequel we simply restrict our attention to situations in which it does exist.

We further assume that  $\phi(\mathbf{x}, k, \mathbf{e}_i) - e^{-ike_i \cdot \mathbf{x}}$  is square integrable in  $k$ . Then, using the Paley–Wiener theorem, as in Ref. 2, it follows that  $\check{\phi}(\mathbf{x}, t, \mathbf{e}_i) = \mathcal{F}^{-1}\{\phi(\mathbf{x}, k, \mathbf{e}_i)\}$  has support in  $t$  in the interval  $[-\mathbf{e}_i \cdot \mathbf{x}, \mathbf{e}_i \cdot \mathbf{x}]$  (compare this to the one-dimensional support interval  $[-x, x]$ ). Thus  $\phi(\mathbf{x}, k, \mathbf{e}_i)$  has the Povsner–Levitan representation [compare with (7.3) in Ref. 2 and (2.14) above]

$$\phi(\mathbf{x}, k, \mathbf{e}_i) = e^{-ike_i \cdot \mathbf{x}} - \int_{-\mathbf{e}_i \cdot \mathbf{x}}^{\mathbf{e}_i \cdot \mathbf{x}} m(\mathbf{x}, t, \mathbf{e}_i) e^{-ikt} dt \quad (3.6)$$

[the impulse in the  $-\mathbf{e}_i \cdot \mathbf{x}$  direction is included in  $\phi(\mathbf{x}, k, -\mathbf{e}_i)$ ] so that  $m(\mathbf{x}, t, \mathbf{e}_i)$  is the nonimpulsive part of

the regular solution  $\check{\phi}(\mathbf{x}, t, \mathbf{e}_i)$ . Note that in the time domain, the solutions  $\check{\phi}(\mathbf{x}, t, \mathbf{e}_i)$  and  $\psi(\mathbf{x}, t, \mathbf{e}_i)$  have complementary support in that the former has support in  $t$  on the interval  $[-\mathbf{e}_i \cdot \mathbf{x}, \mathbf{e}_i \cdot \mathbf{x}]$ , while the latter has support in  $t$  on the interval  $[\mathbf{e}_i \cdot \mathbf{x}, \infty]$ .

The solutions  $\psi(\mathbf{x}, k, \mathbf{e}_i)$  and  $\phi(\mathbf{x}, k, \mathbf{e}_i)$  are related by a Jost operator  $J(k)$ . This is an operator on the space  $L^2(S^2)$  ( $S^2$  is the unit sphere) with kernel  $J(k, \mathbf{e}_1, \mathbf{e}_2)$ . The  $2 \times 2$  matrix multiplication (2.5) becomes

$$\phi(\mathbf{x}, k, \mathbf{e}_i) = \int_{S^2} \psi(\mathbf{x}, k, \mathbf{e}_s) J(k, \mathbf{e}_s, \mathbf{e}_i) d\mathbf{e}_s. \quad (3.7)$$

The Jost operator has inverse  $J^{-1}(k)$  with a kernel defined as above. Setting  $\mathbf{x} = \mathbf{0}$  results in

$$\begin{aligned} \psi(\mathbf{0}, k, \mathbf{e}_i) &= \int_{S^2} \phi(\mathbf{0}, k, \mathbf{e}_s) J^{-1}(k, \mathbf{e}_s, \mathbf{e}_i) d\mathbf{e}_s \\ &= \int_{S^2} J^{-1}(k, \mathbf{e}_s, \mathbf{e}_i) d\mathbf{e}_s = \mathbf{1} J^{-1}(k), \end{aligned} \quad (3.8)$$

where the effect of the operator  $\mathbf{1}$  is a generalization of pre-multiplication by the vector  $[1, 1]$  in (2.7). This confirms that the Jost operator defined here matches the one defined in Ref. 2.

In Sec. II the potential was required to have support in the half-space  $x > 0$ , allowing an explicit representation (2.8) of the Jost function to be determined. Unfortunately, this will not work for the three-dimensional problem, since the present problem is defined over all of  $\mathbb{R}^3$ . It is noted in Ref. 2 that the Jost operator satisfies

$$J(-k) = QS(k)J(k)Q, \quad (3.9)$$

where  $S(k)$  is the scattering operator with kernel

$$S(k, \mathbf{e}_s, \mathbf{e}_i) - I = -(k/2\pi i)A(k, \mathbf{e}_s, \mathbf{e}_i) \quad (3.10)$$

and  $Q$  is the operator such that  $QA(k, \mathbf{e}_s, \mathbf{e}_i) = A(k, -\mathbf{e}_s, \mathbf{e}_i)$ . In Ref. 2 the relation (3.9) leads to a Marchenko integral equation for the kernel  $J(k, \mathbf{e}_s, \mathbf{e}_i)$ . We now derive a similar equation for the kernel  $J^{-1}(k, \mathbf{e}_s, \mathbf{e}_i)$ .

From (3.9) we have that

$$J^{-1}(-k) = QJ^{-1}(k)S^H(k)Q, \quad (3.11)$$

where the well-known unitarity of the scattering operator  $S(k)$  has been used. Repeating the derivation of Ref. 2 (p. 1707) for (3.11) instead of (3.9) leads to a Marchenko integral equation for the kernel  $J^{-1}(k, \mathbf{e}_s, \mathbf{e}_i)$ , as follows. Since both  $\psi$  and  $\phi$  contain impulses in the time domain,  $J^{-1}$  does also, and  $J^{-1}(k) - 1$  is square integrable (see Ref. 2). Therefore we may write

$$J^{-1}(k, \mathbf{e}_s, \mathbf{e}_i) = 1 + \int_0^\infty L(t, \mathbf{e}_s, \mathbf{e}_i) e^{-ikt} dt \quad (3.12)$$

and, following Ref. 2, this leads to the following Marchenko integral equation for  $L(t, \mathbf{e}_s, \mathbf{e}_i)$ :

$$\begin{aligned} L(t, \mathbf{e}_s, \mathbf{e}_i) &= G(t, -\mathbf{e}_s, \mathbf{e}_i) \\ &+ \int_0^\infty \int_{S^2} L(\tau, -\mathbf{e}_s, \mathbf{e}') G(t + \tau, \mathbf{e}', \mathbf{e}_i) d\mathbf{e}' d\tau, \end{aligned} \quad (3.13)$$

where  $G(t, \mathbf{e}_i, \mathbf{e}_s)$  is defined by

$$\begin{aligned} G(t, \mathbf{e}_i, \mathbf{e}_s) &= \frac{1}{2\pi} \int_{-\infty}^\infty (S(k, \mathbf{e}_s, -\mathbf{e}_i) - 1) e^{ikt} dk \\ &= \frac{1}{4\pi^2} \int_{-\infty}^\infty ikA(k, \mathbf{e}_s, -\mathbf{e}_i) e^{ikt} dk \end{aligned} \quad (3.14)$$

(note the transposition of  $\mathbf{e}_i$  and  $\mathbf{e}_s$  caused by the Hermitian operator).

It is indeed unfortunate that the solution of the generalized Gel'fand-Levitan equation requires the prior solution of this Marchenko equation in order to obtain the inverse Jost operator kernel  $J^{-1}(k, \mathbf{e}_s, \mathbf{e}_i)$ , but there is no other known way to obtain this kernel. However, in Sec. III C below it will be shown that the generalized Marchenko equation for the scattered field resulting from a reflection problem can be derived from (3.13) and (3.14).

## B. Orthonormalization

It is well known that in the absence of bound states the solutions  $\psi(\mathbf{x}, k, \mathbf{e}_i)$  are orthonormal, in that

$$\begin{aligned} \frac{1}{(2\pi)^3} \int_0^\infty \int_{S^2} \psi(\mathbf{x}, k, \mathbf{e}) \psi^*(\mathbf{y}, k, \mathbf{e}) k^2 d\mathbf{e} dk \\ = \delta(\mathbf{x} - \mathbf{y}). \end{aligned} \quad (3.15)$$

As in the one-dimensional case, the solutions  $\{\psi(\mathbf{x}, k, \mathbf{e}_i)\}$  are inappropriate candidates for the result of an orthogonalization procedure, since they are initiated in the far field. The solutions  $\{\phi(\mathbf{x}, k, \mathbf{e}_i)\}$  are ideal candidates for such a procedure, since they are generated in increasing  $|\mathbf{e}_i \cdot \mathbf{x}|$  in the time domain, and from (3.6) and (3.15) they are orthonormal with respect to the inner product

$$\begin{aligned} \langle u_1(\mathbf{x}, k, \mathbf{e}), u_2(\mathbf{y}, k, \mathbf{e}) \rangle \\ = \frac{1}{(2\pi)^3} \int_0^\infty \int_{S^2} \int_{S^2} u_1(\mathbf{x}, k, \mathbf{e}_1) (J^H J)^{-1}(k, \mathbf{e}_1, \mathbf{e}_2) \\ \times u_2^*(\mathbf{y}, k, \mathbf{e}_2) k^2 d\mathbf{e}_1 d\mathbf{e}_2 dk. \end{aligned} \quad (3.16)$$

However, the region  $\{\mathbf{y} \in \mathbb{R}^3: -\mathbf{e}_i \cdot \mathbf{x} \leq \mathbf{e}_i \cdot \mathbf{y} \leq \mathbf{e}_i \cdot \mathbf{x}\}$  in which the orthogonalization takes place is still not compact, so a further transformation is necessary. Since the time-domain solution  $\check{\phi}(\mathbf{x}, t, \mathbf{e}_i)$  is only defined for  $t > 0$ , we may regard its smooth part  $m(\mathbf{x}, t, \mathbf{e}_i)$  as the Radon transform of a function  $h(\mathbf{x}, \mathbf{y})$  (Ref. 2):

$$\begin{aligned} \mathcal{R}\{h(\mathbf{x}, \mathbf{y})\} &= \int h(\mathbf{x}, \mathbf{y}) \delta(t - \mathbf{e}_i \cdot \mathbf{y}) d\mathbf{y} \\ &= m(\mathbf{x}, t, \mathbf{e}_i) \operatorname{sgn}[\mathbf{e}_i \cdot \mathbf{x}]. \end{aligned} \quad (3.17)$$

Note that the support of  $h(\mathbf{x}, \mathbf{y})$  in  $\mathbf{y}$  is the interior of the sphere of radius  $|\mathbf{x}|$ :  $\{|\mathbf{y}| < |\mathbf{x}|\}$ . This is the triangularity property that makes an integral equation procedure possible; we see here that this property follows from time causality. Using the projection-slice property of the Radon transform, the Fourier transform relation (3.6) becomes

$$\begin{aligned} \phi(\mathbf{x}, k, \mathbf{e}_i) &= e^{-ike_i \cdot \mathbf{x}} - \int h(\mathbf{x}, \mathbf{y}) e^{-ike_i \cdot \mathbf{y}} d\mathbf{y} \\ &= \mathcal{F}\{\delta(\mathbf{x} - \mathbf{y}) - h(\mathbf{x}, \mathbf{y})\}. \end{aligned} \quad (3.18)$$

From this point on the argument matches that given in Sec. II for the one-dimensional problem. The free-space so-

lutions  $\{e^{-ike_r \mathbf{x}}\}$  are orthogonalized in increasing  $|\mathbf{x}|$ . The projection of  $e^{-ike_r \mathbf{x}}$  on  $\text{span}\{\phi(\mathbf{y}, k, \mathbf{e}_i), |\mathbf{y}| < |\mathbf{x}|\}$  =  $\text{span}\{e^{-ike_r \mathbf{y}}, |\mathbf{y}| < |\mathbf{x}|\}$  takes the form [compare to (2.14)]

$$\mathcal{P} = \int_{|\mathbf{y}| < |\mathbf{x}|} h(\mathbf{x}, \mathbf{y}) e^{-ike_r \mathbf{y}} d\mathbf{y}. \quad (3.19)$$

The reason that the kernel of the projection (3.19) is  $h(\mathbf{x}, \mathbf{y})$  is as follows. As in the one-dimensional case, we take the error

$$e^{-ike_r \mathbf{x}} - \mathcal{P} = e^{-ike_r \mathbf{x}} - \int_{|\mathbf{y}| < |\mathbf{x}|} h(\mathbf{x}, \mathbf{y}) e^{-ike_r \mathbf{y}} d\mathbf{y} = \phi(\mathbf{x}, k, \mathbf{e}_i) \quad (3.20)$$

to be the regular solution at  $\mathbf{x}$ , since by the orthogonality principle the error is orthogonal to this subspace, and thus may be used to expand it. Comparing (3.18) and (3.20) proves that the kernel of the projection (3.19) is precisely  $h(\mathbf{x}, \mathbf{y})$ . The kernel  $h(\mathbf{x}, \mathbf{y})$  should be compared with the matrix kernel  $M(\mathbf{x}, \mathbf{y})$  in the projection (2.14). The difference is that  $h(\mathbf{x}, \mathbf{y})$  is the *inverse Radon transform* of the smooth part of the regular solution in the time domain, while  $M(\mathbf{x}, \mathbf{y})$  is simply the smooth part of the regular solution in the time domain.

We now derive a generalized Gel'fand–Levitan integral equation identical to that of Ref. 2. For convenience the notation of Ref. 2 is adopted. Writing out the condition that the error  $\phi(\mathbf{x}, k, \mathbf{e}_i)$  be orthogonal to the subspace element  $e^{-ike_r \mathbf{y}}$  for  $|\mathbf{y}| \leq |\mathbf{x}|$ , with respect to the inner product defined by (3.16), results in

$$h_0(\mathbf{x}, \mathbf{y}) = h(\mathbf{x}, \mathbf{y}) + \int_{|\mathbf{z}| < |\mathbf{x}|} h(\mathbf{x}, \mathbf{z}) h_0(\mathbf{z}, \mathbf{y}) d\mathbf{z}, \quad (3.21)$$

which is Eq. (8.4) in Ref. 2. Here

$$h_0(\mathbf{x}, \mathbf{y}) = \frac{1}{(2\pi)^3} \int_0^\infty \int_{S^2} \int_{S^2} M(k, \mathbf{e}_1, \mathbf{e}_2) \times e^{-ik(\mathbf{e}_1 \cdot \mathbf{x} - \mathbf{e}_2 \cdot \mathbf{y})} k^2 d\mathbf{e}_1 d\mathbf{e}_2 dk = \mathcal{F}_{k, \mathbf{e}_2}^{-1} \int_{S^2} M(k, \mathbf{e}_1, \mathbf{e}_2) e^{-ike_r \mathbf{x}} d\mathbf{e}_1, \quad (3.22)$$

where  $M(k, \mathbf{e}_1, \mathbf{e}_2) = ((J^H J)^{-1} - I)(k, \mathbf{e}_1, \mathbf{e}_2)$  is the perturbation of the spectral function  $(J^H J)^{-1}$  away from its free-space representation. Equations (3.21) and (3.22) should be compared to the one-dimensional problem Eqs. (2.16) and (2.17).

The key fact here is the *triangularity* of  $h(\mathbf{x}, \mathbf{y})$  in (3.21). This follows from the support of the regular solution, although it has also been established rigorously.<sup>19</sup> Taking the *partial inverse Radon transform*<sup>19</sup> of (3.21), and using (3.17) and the projection-slice theorem results in the *generalized Gel'fand–Levitan integral equation*<sup>2</sup>

$$\text{sgn}[\mathbf{e}_i \cdot \mathbf{x}] m(\mathbf{x}, t, \mathbf{e}_i) = \int_{S^2} M(t + \mathbf{e}_i \cdot \mathbf{x}, \mathbf{e}_s, \mathbf{e}_i) d\mathbf{e}_s - \int_{S^2} \int_{-|\mathbf{e}_s \cdot \mathbf{x}|}^{|\mathbf{e}_s \cdot \mathbf{x}|} \text{sgn}[\mathbf{e}_s \cdot \mathbf{x}] \times m(\mathbf{x}, \tau, \mathbf{e}_s) M(t + \tau, \mathbf{e}_s, \mathbf{e}_i) d\tau d\mathbf{e}_s, \quad (3.23)$$

where  $M(t, -\mathbf{e}_s, \mathbf{e}_i) = \mathcal{F}^{-1}\{M(k, \mathbf{e}_s, \mathbf{e}_i)\}$ .

Once the integral equation (3.23) has been solved, the potential  $V(\mathbf{x})$  is then recovered from  $m(\mathbf{x}, t, \mathbf{e}_i)$  using the *miracle*<sup>2</sup> or *fundamental identity*<sup>7</sup>

$$V(\mathbf{x}) = 2\mathbf{e}_i \cdot \nabla m(\mathbf{x}, t = \mathbf{e}_i \cdot \mathbf{x}, \mathbf{e}_i), \quad (3.24)$$

which is the three-dimensional analog of (2.22) and is derived in the same way. Note the sign change in (3.24) as compared to the equation in Refs. 2 and 7; this is due to the use of the regular solution instead of  $\psi(\mathbf{x}, k, \mathbf{e}_i)$ . In Refs. 18 and 19 the gradient of the *jump* in the scattered field must be used in (3.24), since the regular solution as defined in those papers is not known to satisfy  $m(\mathbf{x}, t, \mathbf{e}_i) = 0$  for  $t > \mathbf{e}_i \cdot \mathbf{x}$ . However, in the present case this anticausality follows from the support of the regular solution.

As in the one-dimensional case, the generalized Gel'fand–Levitan equation has a finite interval of integration, which is an advantage over the generalized Marchenko integral equation to be derived next. However, it is necessary to solve the Marchenko equation (3.13) for the generalized Jost function  $J^{-1}(k, \mathbf{e}_1, \mathbf{e}_2)$  first, which is most inconvenient.

### C. Generalized Marchenko equation

In the one-dimensional case the inverse Jost function was related to the reflection problem scattered field at the origin by (2.7). Since the scattered field was known at the origin, an explicit representation of  $J^{-1}$  could be found. For the three-dimensional case, the reflection problem scattered field is not known at the origin, and  $J^{-1}$  must be found from the integral equation (3.13). However, the integral equation (3.13) can be transformed into an integral equation for the scattered field at the origin, and then into an integral equation for the reflection problem scattered field *anywhere*, using an observation made in Ref. 2. This integral equation is identical to the generalized Marchenko equation of Ref. 2.

Integrating (3.13) with respect to  $\mathbf{e}_s$  over the unit sphere  $S^2$  and using (3.8) and (3.12) results in

$$\check{u}_s(\mathbf{0}, t, \mathbf{e}_i) = \int_{S^2} G(t, \mathbf{e}_s, \mathbf{e}_i) d\mathbf{e}_s + \int_0^\infty \int_{S^2} G(t + \tau, \mathbf{e}', \mathbf{e}_i) \check{u}_s(\mathbf{0}, t - \mathbf{e}' \cdot \mathbf{x}) d\mathbf{e}' d\tau, \quad (3.25)$$

where  $\check{u}_s(\mathbf{0}, t, \mathbf{e}_i)$  is the scattered field at the origin for the reflection problem with probing impulsive plane wave in the direction  $\mathbf{e}_i$ . This integral equation is equivalent to the generalized Marchenko equation of Ref. 2 with  $\mathbf{x} = \mathbf{0}$ , since it is identical to (4.14) of Ref. 7 with  $\mathbf{x} = \mathbf{0}$ . Here  $G(t, \mathbf{e}_i, \mathbf{e}_s)$  is the time derivative of the inverse Fourier transform of the scattering amplitude  $A(k, \mathbf{e}_s, \mathbf{e}_i)$  [note the transposition of  $\mathbf{e}_i$  and  $\mathbf{e}_s$ , and compare with (4.11) of Ref. 7].

We now make use of an observation made in Ref. 2. If the potential  $V(\mathbf{x})$  is *shifted* by a translation  $\mathbf{x}'$ , becoming  $V(\mathbf{x} - \mathbf{x}')$ , then the solution  $\psi(\mathbf{x}, k, \mathbf{e}_i)$  becomes  $\psi(\mathbf{x} - \mathbf{x}', k, \mathbf{e}_i) e^{-ike_r \mathbf{x}'}$  and thus the scattering amplitude  $A(k, \mathbf{e}_i, \mathbf{e}_s)$  becomes  $A(k, \mathbf{e}_i, \mathbf{e}_s) e^{-ik(\mathbf{e}_s - \mathbf{e}_i) \cdot \mathbf{x}'}$ . Therefore to compute the scattered field  $\check{u}_s(\mathbf{x}', t, \mathbf{e}_i)$  at  $\mathbf{x}'$  resulting from a potential  $V(\mathbf{x})$ , we compute the field at the origin  $\mathbf{x} = \mathbf{0}$  [using (3.25)] resulting from a shifted potential  $V(\mathbf{x} - \mathbf{x}')$ .



This merely requires that we replace the scattering amplitude, and hence  $G(t, \mathbf{e}_i, \mathbf{e}_s)$ , with its shifted version. This yields

$$G(t, \mathbf{e}_i, \mathbf{e}_s, \mathbf{x}) = - (2\pi)^{-2} \int_{-\infty}^{\infty} e^{ik(t - (\mathbf{e}_s - \mathbf{e}_i) \cdot \mathbf{x})} ik A(k, \mathbf{e}_s, \mathbf{e}_i) dk \quad (3.26)$$

and the integral equation (3.25) is modified to

$$\check{v}_s(\mathbf{x}, t, \mathbf{e}_i) = \int_{S^2} G(t, \mathbf{e}_s, \mathbf{e}_i, \mathbf{x}) d\mathbf{e}_s + \int_0^\infty \int_{S^2} G(t + \tau, \mathbf{e}', \mathbf{e}_i, \mathbf{x}) \check{v}_s(\mathbf{x}, t - \tau, \mathbf{e}') d\mathbf{e}' d\tau, \quad (3.27)$$

where

$$\check{v}_s(\mathbf{x}, t, \mathbf{e}_i) = \check{u}_s(\mathbf{x}, t - \mathbf{e}_i \cdot \mathbf{x}, \mathbf{e}_i) \quad (3.28)$$

is simply the delayed scattered field. Equations (3.26) and (3.27) are identical to (4.11) and (4.14) of Ref. 7, which in turn are equivalent to the generalized Marchenko integral equation of Ref. 2.

It has been shown that the generalized Gel'fand-Levitan integral equation of Ref. 2 can be interpreted as an orthogonality condition for the construction of the solutions  $\phi(\mathbf{x}, k, \mathbf{e}_i)$  with respect to the inner product (3.16). The construction of the inverse Jost operator requires the solution of a Marchenko equation, and this equation can be extended to the generalized Marchenko integral equation of Ref. 2. This shows the relation between the two integral equations, and how this relation is a generalization of the relation that exists between them in one dimension.

#### IV. FAST ALGORITHMS FOR THE THREE-DIMENSIONAL INVERSE SCATTERING PROBLEM

In this section differential, layer stripping fast algorithms for solving the three-dimensional inverse scattering problem are presented. These algorithms require fewer computations than solving the integral equations presented above, but they reconstruct  $V(\mathbf{x})$ ,  $\psi(\mathbf{x}, t, \mathbf{e}_i)$ , and  $\phi(\mathbf{x}, t, \mathbf{e}_i)$  just as the integral equations do. They are also generalizations of the algorithms presented in Sec. II.

##### A. The reflection problem

A major distinction between the one-dimensional and three-dimensional reflection problems is that for the one-dimensional problem near-field and far-field data are identical (save for a time shift), while for the three-dimensional problem the extrapolation of the near-field scattered field from the far-field scattering amplitude is a nontrivial problem. For the reflection problem differential algorithms it is assumed that the scattered field is observed in the *near field*. Since in many inverse scattering problems (e.g., inverse seismic problems) data are actually taken in the near field, this assumption is not only tenable, but realistic.

A differential algorithm for solving the reflection problem is as follows.<sup>12</sup> For convenience let  $z = \mathbf{e}_i \cdot \mathbf{x}$  be the axis normal to the incident impulsive plane wave, and let  $\mathbf{y}$  be the

two directions perpendicular to  $z$ , so that any function  $f(\mathbf{x})$  of  $\mathbf{x}$  can be written as a function  $f(z, \mathbf{y})$  of  $z$  and  $\mathbf{y}$ .

(1) Initialize the algorithm on the plane  $z = \mathbf{e}_i \cdot \mathbf{x} = 0$  with observations of the scattered field and its derivative on this plane.

(2) Propagate the following equations recursively in  $z = \mathbf{e}_i \cdot \mathbf{x}$  and  $t$ , for  $t \geq z$  and for all  $\mathbf{y}$ :

$$\left( \frac{\partial}{\partial z} + \frac{\partial}{\partial t} \right) u(z, \mathbf{y}, t) = q(z, \mathbf{y}, t), \quad (4.1a)$$

$$\left( \frac{\partial}{\partial z} - \frac{\partial}{\partial t} \right) q(z, \mathbf{y}, t) = (V(\mathbf{x}) - \Delta_y) u(z, \mathbf{y}, t), \quad (4.1b)$$

$$V(\mathbf{x}) = -2q(z, \mathbf{y}, t = z), \quad (4.1c)$$

where  $\Delta_y$  is the Laplacian operator with respect to  $\mathbf{y}$ , which is also the *transverse* Laplacian operator with respect to  $\mathbf{x}$ . The recursion patterns for this algorithm are the same as for its one-dimensional counterpart, and are illustrated in Fig. 4.

Note that (4.1c) follows using the same argument used to derive (3.24) (see Ref. 12) and is comparable to (2.22). Also note that this algorithm requires  $O(N^6)$  operations to reconstruct  $V(\mathbf{x})$ , while the solution of the generalized Marchenko integral equation requires  $O(N^{12})$  operations. Some details on ways to implement this algorithm numerically are given in Ref. 12.

The computational simplicity of this algorithm as compared to the solution of the generalized Marchenko integral equation (and the algorithm for the regular problem given below) results from the inherent causal structure of the reflection problem, which is fully exploited by this algorithm. Instead of attempting to reconstruct the scattered field all at once in one huge operation, the algorithm recursively reconstructs both the scattered field and the potential as the wave front penetrates the region where  $V(\mathbf{x})$  has support. It then strips away the effects of the reconstructed region, reducing the size of the problem and obviating the need to store information about the reconstructed region to process the data associated with the unknown region. Another important feature is the use of near-field data, which avoids the coupling between the scattered fields associated with different  $\mathbf{e}_i$  that makes the generalized Marchenko equation so computationally intensive to solve.

##### B. The regular problem

The regular problem lacks the causal structure of the reflection problem, which is why it is harder to solve using either the generalized Gel'fand-Levitan equation or a differential algorithm. Two different differential algorithms for the regular problem are presented. The second algorithm is similar to an algorithm proposed for estimation of random fields in Ref. 13, illustrating some connections between inverse scattering in three dimensions and estimation of random fields. This generalizes the connections between these two topics that exists in one dimension (e.g., Ref. 20).

A new differential algorithm for solving the regular problem is as follows.

(1) Initialize the algorithm on the plane  $z = \mathbf{e}_i \cdot \mathbf{x} = 0$  using

$$m(z = 0, \mathbf{y}, t = 0) = n(z = 0, \mathbf{y}, t = 0) = 0. \quad (4.2)$$

(2) Propagate the following equations recursively in  $z$  and  $t$ , for  $-z \leq t \leq z$  and for all  $y$ :

$$\left(\frac{\partial}{\partial z} + \frac{\partial}{\partial t}\right)m(z,y,t) = n(z,y,t), \quad (4.3a)$$

$$\left(\frac{\partial}{\partial z} - \frac{\partial}{\partial t}\right)n(z,y,t) = (V(x) - \Delta_y)m(z,y,t), \quad (4.3b)$$

$$m(z,y,t = -z) = 0, \quad (4.3c)$$

$$V(x) = 2n(z,y,t = z) \quad (4.3d)$$

obtained from (3.23). The recursion patterns for this algorithm are the same as for its one-dimensional counterpart, and are illustrated in Fig. 3. Note that  $n(z,y,t = z)$  for the regular problem must be obtained from the values of  $n(z,y,t \neq z)$  using the integral equation (3.23). This is analogous to (2.26d) for the one-dimensional problem, for which  $n(x,t = x)$  is obtained from the integral equation (2.20).

Aside from the computation of (4.3d), a major problem with this algorithm is that the region in which the computations are to be carried out has infinite extent in  $y$ . This can be avoided by using the inverse Radon transform, as in (3.15), which maps the region in which computations are performed into the interior of a sphere. Taking the inverse Radon transform of the Schrödinger equation (3.1) in the time domain and using (3.18) results in

$$(\Delta_x - \Delta_y)h(x,y) = V(x)h(x,y), \quad (4.4)$$

where  $\Delta_x$  is again the Laplacian operator with respect to  $\mathbf{x}$ . An equation similar to (4.4) was encountered in the problem of deriving a fast algorithm for the linear least-squares estimation of a homogeneous random field,<sup>13</sup> and a variation of the algorithm presented in Ref. 13 is useful here.

Another differential algorithm for solving the regular problem is as follows.

(1) Initialize the algorithm at the origin using

$$h(0,0) = g(0,0) = 0. \quad (4.5)$$

(2) Propagate the following equations recursively in  $r = |\mathbf{x}|$  and  $s = |\mathbf{y}|$ , for  $0 \leq s \leq r$ :

$$\left(\frac{\partial}{\partial r} + \frac{\partial}{\partial s}\right)h(x,y) = g(x,y), \quad (4.6a)$$

$$\left(\frac{\partial}{\partial r} - \frac{\partial}{\partial s}\right)g(x,y) = H(x,y), \quad (4.6b)$$

$$H(x,y) = V(x)h(x,y) + (\Delta_y^0 - \Delta_x^0)h(x,y), \quad (4.6c)$$

$$h(x,0) \text{ obtained from } \frac{\partial}{\partial s}h(x,y = 0) = 0, \quad (4.6d)$$

$$V(x) = -2g(x,|y| = |\mathbf{x}|)/r^2 \quad (4.6e)$$

is obtained from (3.21).

Here  $\Delta_x^0$  is the transverse radial Laplacian operator in spherical coordinates, which is

$$\Delta_x^0 = \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}. \quad (4.7)$$

The quantity  $h(x,y)$  being computed in this algorithm is actually  $rsh(x,y)$ , where  $h(x,y)$  is defined in (3.20) as the inverse Radon transform of the scattered field  $m(x,t,e_i)$ . Multiplication by  $rs = |\mathbf{x}| |\mathbf{y}|$  is a normalization that results in better numerical behavior near the origin.

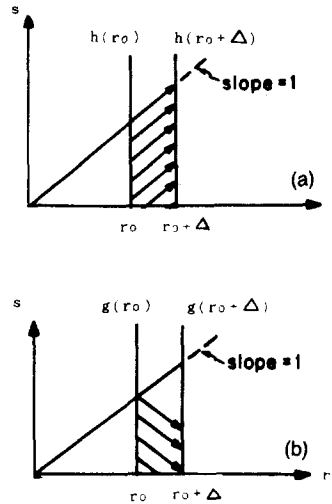


FIG. 5. (a) Recursion pattern for updating  $h(r,s)$  in the fast algorithm for the 3-D regular problem. (b) Recursion pattern for updating  $g(r,s)$  in the fast algorithm for the 3-D regular problem.

The recursion pattern for this algorithm is illustrated in Fig. 5. Note that since the radii  $r$  and  $s$  are both non-negative, the recursion pattern differs from the previous algorithm in that  $s$  is required to be non-negative. The only other significant difference is that computations need only be performed over the interior of the sphere of radius  $r$ , rather than over the infinite slab  $-e_i \cdot \mathbf{x} \leq t \leq e_i \cdot \mathbf{x}$ . This is a considerable advantage over the two preceding algorithms, both of which require computations over an infinite region in  $y$ . However, (4.6e) still requires a considerable amount of computation at each recursion, although now the simpler integral equation (3.21) is used to compute  $g(x,|\mathbf{x}|)$  from values of  $g(x,y)$ . This computation is absent in the reflection problem algorithm, since this problem has a causal structure that is more easily exploited.

The amount of computation required by the above algorithm for the regular problem is  $O(N^8)$  operations. This is a significant reduction from the  $O(N^{12})$  operations required to solve the generalized Gel'fand-Levitan integral equation. Note that the ratio of the exponents of the orders of computations required for the integral equation procedure to the differential procedure is the same in both one and three dimensions, viz.,  $\frac{12}{8} = \frac{3}{2}$ . Also note that the layer stripping algorithm for the reflection problem requires only  $O(N^6)$  computations. This is because the layer stripping reflection problem algorithm is initialized using near-field data, while the regular problem procedures all use far-field data in the form of the scattering amplitude [in order to compute the Jost function  $J(k)$ ].

This algorithm is quite similar to the algorithm given in Ref. 13 for computation of the optimal filter for the linear, least-squares estimation of a homogeneous random field. Since the integral equation (3.21) looks much like a multidimensional Wiener-Hopf equation, this is not surprising. The form of (3.21) suggests that the well-known connection between inverse scattering and linear least-squares estimation that exists in one dimension<sup>20</sup> extends to higher dimensions. Details of this connection are given in Ref. 21 for iso-

tropic random fields and spherically symmetric potentials, and in Ref. 22 for a more general class of random fields and nonspherically symmetric potentials.

## V. CONCLUSION

This paper has presented a unified treatment of various differential and integral equation procedures for solving three-dimensional inverse scattering problems. The relation between the generalized Gel'fand-Levitan and Marchenko integral equations of Ref. 2 has been explored by noting that the former can be interpreted as an orthogonality principle with respect to an inner product defined in terms of a weighting function computed using an integral equation equivalent to the latter. The problems solved by the two integral equations, and the resulting scattering solutions, are complementary in their support. This is emphasized by the differential counterparts to the integral equation procedures, which require less computation since they directly exploit the causal structure of the inverse scattering problem.

An important feature of this presentation is the emphasis on how results for the one-dimensional inverse problem generalize to three dimensions. The parallels between Secs. II and III are remarkable, considering the greater complexity of the three-dimensional problem. These strong parallels in the derivations of both the integral equation procedures and their differential, fast algorithm counterparts suggest that the approach taken in this paper may be particularly insightful for further research.

Several topics developed in this paper require further research. The most important one is the connection between multidimensional inverse scattering and linear least-squares estimation of random fields. A useful starting point would be the characterization of the class of covariance functions that can be put in the form of (3.22). Connections between other exact inverse problem procedures and those of Ref. 2 should also be explored, in the spirit of Ref. 9; this could result in further insights and more fast algorithms. Finally, the numerical performances of all of these procedures need to be investigated.

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