CONNECTION BETWEEN TIME- AND FREQUENCY-DOMAIN THREE-DIMENSIONAL INVERSE PROBLEMS FOR THE SCHRÖDINGER EQUATION

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INTRODUCTION

The use of inverse scattering methods in electromagnetic remote sensing, seismic exploration and ultrasonic imaging is rapidly expanding. For these cases which involve classical wave equations with variable velocity,[1] no exact inversion methods exists for general three-dimensional (3d) scatterers. However, exact inversion methods (for example, those based on the Born series[2] and the Newton-Marchenko equation[2]) do exist for the 3d Schrödinger equation. In this paper, these inversion methods for Schrödinger's equation will be rewritten in a form which brings out certain analogies with classical wave equations. It is hoped these analogies will eventually contribute to a common exact inversion method for both types of equations.

The manner in which one-dimensional (1d) inversion methods developed provides hope for the program outlined above. Exact inversion methods for the 1d Schrödinger equation have been known for some time.[2] For broad classes of potentials, these varied inverse methods can be described in a common way in terms of simple "layer stripping" algorithms.[3-5] Many authors have contributed importantly to the solution of the 1d inverse problem[6,7]. References 3-5 provide citations to many of the recent important results. An important historical element in the discovery of "layer-stripping" methods was the development of the "time-domain" Marchenko equation.[8] Inversion methods for many 1d classical wave equations were found by first reducing them to the Schrödinger equation and then using the Marchenko equation.

From our point of view, at least three ideas were essential in the historical unification of 1d inversion methods. First, the various problems (including Schrödinger's equation for a broad class of potentials) may be expressed as "time-domain" hyperbolic wave equations. Second, the potential can be determined from the propagation of the initial wavefront. Finally, Marchenko's equation provides an important link between the methods.

The purpose of this paper is to re-express these three ideas for the three-dimensional case. First, it will be shown that for 3d repulsive potentials with compact support, the time independent Schrödinger equation may be related to a "time-domain" hyperbolic wave equation. Next, work relating the potential to the wavefront is reviewed. Then, the "time-domain" Newton-Marchenko inverse scattering equations are given for this hyperbolic wave equation. Finally, the implications of these results for the classical wave equation are briefly discussed.

"TIME-DOMAIN" QUANTUM SCATTERING[9]

Three-dimensional quantum scattering theory starts from the time-independent Schrödinger equation

$$(\Delta + k^2 - V)\psi = 0 \quad . \tag{1}$$

Here Δ is the Laplacian and V is a real-valued function, which in this paper we will take to be smooth, positive and of compact support. Thus, we assume that V gives rise to no bound states. Scattering solutions of Eq. (1) are determined by the Lippmann-Schwinger equation

$$\psi^{\pm}(k,\hat{e},\vec{x}) = \exp(ik\hat{e}\cdot\vec{x}) + \int G_0^{\pm}(k,|\vec{x}-\vec{y}|)V(\vec{y})\psi^{\pm}(k,\hat{e},\vec{y})d\vec{y} \tag{2}$$

where $\hat{e}$ is a unit vector denoting the direction of incidence and k is a scalar variable denoting the magnitude of the wavevector. Also,

$$G_0^{\pm}(k,r) = -(4\pi r)^{-1} \exp(\pm ikr) \quad . \tag{3}$$

The + sign corresponds to the outgoing radiation condition, while the - sign corresponds to the incoming radiation condition. Examination of Eq. (2) shows that ψ^+ and $\psi-$ are related via

$$\psi^-(k,\hat{e},\vec{x}) = \psi^+(-k,-\hat{e},\vec{x}) \tag{4}$$

and

$$\psi(k,\hat{e},\vec{x}) = \psi^*(-k,\hat{e},\vec{x}) \tag{5}$$

where the star indicates complex conjugate. We write the outgoing wavefunction as

$$\psi^+(k,\hat{e}_i,\vec{x}) = \exp(ik\hat{e}_i\cdot\vec{x}) + |x|^{-1} A(k,\hat{e}_s,\hat{e}_i) \exp(ik|\vec{x}|) + h(k,\hat{e}_i,\vec{x}) \tag{6}$$

where $\vec{x} = |\vec{x}|\hat{e}_s$ and A is the scattering amplitude

$$A(k,\hat{e}_s,\hat{e}_i) = -(4\pi)^{-1} \int \exp(-ik\hat{e}_s\cdot\vec{x})V(\vec{x})\psi(k,\hat{e}_i,\vec{x})d\vec{x} \quad . \tag{7}$$

It can be shown that for each k, the remainder $h(k,\hat{e},\vec{x})$ is a uniformly square-integrable function of $\vec{x}$.

A time-independent equation such as (1) can be related to equations in the time domain. We shall use the Fourier transform

$$f(t) = (2\pi)^{-1} \int_{-\infty}^{\infty} \exp(-ikt)f(k)dk \tag{8}$$

to obtain from (1) the plasma wave equation

$$[\Delta - (\partial^2/\partial t^2) - V(x)]u = 0 \tag{9}$$

where $u = \hat{\psi}$. We have thus transformed (1) into a hyperbolic equation. In our treatment, the constant phase velocity is set equal to one. Note the "time-domain" here is not the physical time associated with the Schrödinger equation, rather it is the formal transform variable defined by Eq. (8). The circumflex is used both to denote unit vectors and Fourier transformed quantities. The solutions of (9) that interest us are those that correspond to Schrödinger's scattering solutions, namely those defined by the formal analog of the Lippmann-Schwinger equation (2)

$$u^{\pm}(t,\hat{e},\vec{x}) = \delta(t-\hat{e}\cdot\vec{x}) + \iint G_0^{\pm}(t-t',|\vec{x}-\vec{y}|)V(\vec{y})u^{\pm}(t',\hat{e},\vec{y})dt'd\vec{y} \tag{10}$$

where

$$G_0^{\pm}(t,r) = -\delta(r\mp t)(4\pi r)^{-1} \tag{11}$$

and

$$u^{\pm}(t,\hat{e},\vec{x}) = (2\pi)^{-1}\int_{-\infty}^{\infty} \exp(-ikt)\psi^{\pm}(k,\hat{e},\vec{x})dk \quad . \tag{12}$$

In writing (12), we have extended the wavefunction ψ to negative values of k via (5). As in the frequency domain, the outgoing solution u^+ and the incoming solution u^- are related by

$$u^-(t,\hat{e},\vec{x}) = u^+(-t,-\hat{e},\vec{x}) \quad . \tag{13}$$

The time-domain integral equation can be used to describe a scattering experiment as follows. At large negative times, the system is prepared with an incident pulse $u°(t,\hat{e},\vec{x}) = \delta(t-\hat{e}\cdot\vec{x})$, propagating along the $\hat{e}$ direction. Because the potential has compact support, the (distributional) solution of (9) for large negative times is identically equal to $\delta(t-\hat{e}\cdot\vec{x})$. This stipulation takes the place of both initial conditions for (9), so that $(\partial/\partial t)u° = \delta'$ for large negative times. The incident field then collides with the target in the neighborhood of the origin and scatters in an outgoing wave plus the incident pulse propagating in the forward direction. After the collision of u° with the potential, the field is measured, typically on a large sphere enclosing the origin. These measurements are the scattering data from which we will infer the potential.

The far-field scattered wave can be described by the impulse response function, R, which is defined to be

$$R(\hat{e}_i,\hat{e}_s\tau) = \lim_{t,|\vec{x}|\to\infty} |\vec{x}|(u(t,\hat{e}_i,\vec{x}) - \delta(t-\hat{e}_i\cdot\vec{x})) \tag{14}$$

where $\tau = t-|\vec{x}|$ and the scattering direction is given by $\hat{e}_s = \vec{x}/|\vec{x}|$. The impulse response function can be expressed explicitly in terms of the potential and the field u by using Eq. (10). We carry out the t-integration and use

$$|\vec{x}-\vec{y}| = |\vec{x}| - \hat{e}_s \cdot \vec{y} + O(|\vec{x}|^{-1}) \quad ,$$

obtaining

$$R(\hat{e}_i,\hat{e}_s,t) = -(4\pi)^{-1} \int u^+(t+\hat{e}_s \cdot \vec{y},\hat{e}_i,\vec{y})V(\vec{y})d\vec{y} \quad . \tag{15}$$

This formula shows that the impulse response is precisely the Fourier transform of the scattering amplitude

$$R(\hat{e}_i,\hat{e}_s,t) = (2\pi)^{-1} \int \exp(-ikt)A(k,\hat{e}_s,\hat{e}_i)dk \quad . \tag{16}$$

The wavefunctions $\psi^{\pm}$ form a complete set in the sense that they give rise to an eigenfunction expansion, which is a decomposition of an L^2 function f in terms of the ψ's. Expressed in the time-domain, this decomposition provides a generalization of Radon's transform as discussed in Ref. 9.

POTENTIAL AND THE WAVEFRONT

The fact that the potential can be related to the jump at the wavefront ($t = \hat{e}\cdot\vec{x}$) was first discussed, so far as we know, by Balanis[8] for the 1d case in 1972. This crucial identity (to be called the fundamental identity from here on) has been discussed for the 3d case by Morawetz,[10] Callias and Uhlmann,[11] and by DeFacio and Rose.[12]

The fundamental identity is based on the progressing wave expansion

$$u(t,\hat{e},\vec{x}) = \delta(t-\hat{e}\cdot\vec{x}) + B(\hat{e},\vec{x})H(t-\hat{e}\cdot\vec{x}) + D(\hat{e},\vec{x})E(t-\hat{e}\cdot\vec{x}) + F(t,\hat{e},\vec{x}) \tag{17}$$

where H is the Heaviside function [$H(x) = 1$, $x>0$ and $H(x) = 0$, $x<0$], $E(s)$ is $sH(s)$, and F is a continuously differentiable function that is zero for $t < \hat{e}\cdot\vec{x}$, and B and D are as yet undetermined. The heuristic principle underlying this expansion is that high frequency signals are not scattered much by the potential.

The transport equations for the PWE are then determined by substituting Eq. (17) into (9) and equating orders of singularity. The terms proportional to δ'' and δ' are identically zero. The term proportional to δ yields

$$V(\vec{x}) = -2e\cdot\nabla B(\hat{e},\vec{x}) \tag{18a}$$

which can also be written

$$V(\vec{x}) = -2\hat{e}\cdot\nabla \lim_{t\to\hat{e}\cdot\vec{x}^+} [u(t,\hat{e},\vec{x}) - \delta(t-\hat{e}\cdot\vec{x})] \quad . \tag{18b}$$

This simple equation will be referred to as the fundamental identity. It is an expression of the fact that Eq. (9) is independent of the variable $\hat{e}$, which we have introduced in the boundary conditions. The fundamental identity relates the potential to the jump in the scattered field at the wavefront; if we knew this jump in the field for all points $\vec{x}$ (including points within the support of the potential), we could reconstruct V from Eq. (18). Of course, in general, the field cannot be measured within the support of the potential. However, the Newton-Marchenko equation which will be discussed in the next section provides a means of computing the wave field within the support of V from the impulse response function.

Integrating Eq. (18) over a line parallel to the direction of incidence yields

$$B(\hat{e},\vec{x}_o) = -\frac{1}{2}\int_{-\infty}^{z_o} V(\vec{x})dz \quad . \tag{19}$$

Here $z = \hat{e}\cdot\vec{x}$ and $\vec{x}_o = (x_o,y_o,z_o)$. Equation (19) indicates that the jump in the wave field at the characteristic surface ($t = \hat{e}\cdot\vec{x} = z_o$) is proportional to the line integral $(-\infty,z_o)$ of the potential. This allows the statement of an exact near field inversion method closely related to the inversion of the Born series. See Ref. 9 for detail.

"TIME-DOMAIN" NEWTON-MARCHENKO EQUATION

The third crucial idea for the 1d problem was the interpretation of Marchenko's equation in the time-domain for the plasma wave equation. The authors have carried out a careful treatment of the time-domain Newton-Marchenko equation for three-dimensional potentials using the plasma wave equation.[9] The resulting time-domain Newton-Marchenko equation is now quoted. For $t > \hat{e}\cdot\vec{x}$

$$\begin{aligned} u^{sc}(t,\hat{e},\vec{x}) &= -\frac{1}{2\pi}\int_{S^2}\left(\frac{\partial}{\partial t}\right)R(\hat{e},\hat{e}',t-\hat{e}'\cdot\vec{x})d^2\hat{e}' \\ &\quad -\frac{1}{2\pi}\int_{S^2}\int_{\hat{e}'\cdot\vec{x}}^{\infty} u^{sc}(\tau,-\hat{e}',\vec{x})\left(\frac{\partial}{\partial t}\right) \\ &\quad \times R(\hat{e},\hat{e}',t+\tau)d\tau d^2\hat{e}' \quad . \end{aligned} \tag{20}$$

For the plasma wave equation, the inversion method is now easily stated. First, the impulse response function, R, is measured for all t, $\hat{e}$, and $\hat{e}'$. Supposing R is the result of scattering from some local potential, Eq. (20) is solved by iteration to yield the scattered field. The value of the potential is then extracted from the jump at the wavefront using Eq. (18).

CLASSICAL WAVE EQUATION: ANALOGIES

The three crucial ideas discussed in this paper are compared and contrasted for the classical and plasma wave equations. The simplest scalar classical wave equation is

$$\left(\Delta - \frac{1}{c^2(\vec{x})}\partial_{tt}\right)u(t,\hat{e},\vec{x}) = 0 \quad . \tag{21}$$

The velocity, $c(\vec{x})$, is assumed to be variable in region of the scatterer. Far from the scatterer, the velocity is assumed to be a constant, c_o. Equation (21) can be brought into a form close to that of the plasma wave equation by defining $V(\vec{x}) = 1/c^2(\vec{x}) - 1/c_o^2$. Then

$$[\,\Delta - \frac{1}{c_o^2}\,(\frac{\partial^2}{\partial t^2}) - V(\vec{x})\,(\frac{\partial^2}{\partial t^2})]\; u(t,\hat{e},\vec{x}) \;=\; 0 \quad . \tag{22}$$

The essential difference between the classical and plasma wave equations is that the potential appears as $V(\vec{x})u$ in Eq. (9) and as $V(\vec{x})\partial_{tt}u$ in Eq. (22). In the frequency domain, $\partial_{tt} \rightarrow -k^2$ corresponds to an energy dependent potential in Eq. (22). As a consequence, abrupt changes in the wavefield (high frequency components) are much more strongly scattered in the classical wave case.

The plasma wave equation becomes weakly scattering at sufficiently high frequencies since $\partial_{tt}u >> Vu$. Consequently, the wavefront is planar and occurs at $t = \hat{e}\cdot\vec{x}$. The wavefront ($-\infty < t < \infty$) passes through all space points $\vec{x}$. Consequently, if $u(t,\hat{e},\vec{x})$ is known, $V(\vec{x})$ is determined from the fundamental identity (Eq. (18)) for all $\vec{x}$.

An analogous result holds for the classical wave equation with important differences. Basically if (1) $u(t,\hat{e},\vec{x})$ is known for an $\vec{x}$ for all t and (2) if a characteristic surface passes through $\vec{x}$, then $V(\vec{x})$ may be determined. This results since the classical wave equation propagates disturbances with the local velocity and without dispersion. Consequently, if a wavefront passes through $\vec{x}$, we may use the time evolution of the sharp delta function at the wavefront to determine the local velocity and thus $V(\vec{x})$.

Differences arise with the PWE as follows. The wavefronts for the classical wave equation do not remain planar as they propagate. Rather they are governed by the Eikonal equations[13] and may distort and even split (caustics). It is quite possible for there to be regions of the potential through which the wavefronts do not pass. If so, the method described above cannot be directly used to determine the potential.

A final and most desirable comparison would be to discuss a 3d generalization of Newton's Marchenko equation to the classical wave equation. Such a generalization is not yet available, however work on it is in progress.

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