A Solution to the Schrödinger Scattering Problem

Jonathan Blackledge
School of Mathematics, Statistics and Computer Science
University of KwaZulu-Natal, South Africa.

Abstract
For a scalar plane wave characterised by wave vector $k$ that is incident upon a scattering potential $r \in \mathbb{R}^3 \mapsto V(r)$, it is shown that an exact scattering solutions exist provided $V(r)$ satisfies the equation
$$\nabla^2 V(r) + 2 \nabla V(r) \cdot \nabla \ln \psi_i(r, k) = 0$$
where $(\nabla^2 + k^2)\psi_i(r, k) = 0$. It is further shown that when $\psi^*_i(r, k) \otimes_r \psi_i(r, k) = \delta^3(r)$ where $\otimes_r$ denotes the convolution integral for $r \in \mathbb{R}^3$ a non-iterative series solution for the scattered field can be established.

Mathematics Subject Classification:
35Q40, 35P25, 74J20, 74J25

Keywords:
Schrödinger scattering, exact scattering solutions, inverse scattering, orthonormal functions.

1 Introduction
The search for exact scattering and inverse scattering solutions has been and continues to be an important field of research in relativistic and non-relativistic quantum mechanics and in electromagnetism, for example. Many papers have reported such solutions for special cases including one-dimensional problems cast in terms of the Gel’fand-Levitan-Marchenko equation, for example ([1]-[4]), and, conditional two- and three-dimensional problems [5], [6].

In the case of certain nonlinear problems associated with the propagation and scattering of solitons and other non-dispersive waves, for example, exact scattering and inverse scattering solution are available [7]. This includes the use of inverse scattering transforms for solving some classes of non-linear partial differential equations including the Korteweg de Vries equation [8], [9], the nonlinear Schrödinger equation, the Sine-Gordon equation and the Toda lattice equation as well as other nonlinear evolution equations [10].

This paper presents an exact scattering solution in any dimension for linear elastic scattering problems associated with scattering potentials that may be
real or complex and frequency dependent. The method is based on expressing the product of the wave function and scattering potential in the form of a convolution of the same wave function and an auxiliary function.

2 Wave Equation

The problem considered in this paper relates to the solution of the equation

\[(\nabla^2 + k^2)\psi(r, k) = V(r)\psi(r, k)\]  

(1)

where \(\nabla^2\) is the Laplacian operator, \(V(r)\) is the scattering potential which may depend on the wave number \(k\) and \(\psi(r, k)\) is the wave function. For Schrödinger scattering problems \(V\) is independent of \(k\) but for Klein-Gordon scattering problems involving spin-less relativistic particles, \(V\) is energy dependent and may be real or complex. In electromagnetism, for a scalar electric field \(\psi\), \(V\) is determined by variations in the relative permittivity and for conductive media is \(k\) dependent and complex. In acoustics, for a scalar pressure field \(\psi\), \(V\) is determined by variations in the compressibility of the material under the assumption that the variations in density are negligible and the effects of absorption due to the viscosity of the medium can be neglected.

3 Fundamental Solution

Equation (1) has a fundamental solution given by the Lippmann-Schwinger equation

\[\psi(r, k) = \psi_i(r, k) + \psi_s(r, k)\]  

(2)

where \(\psi_i\) is the incident wave function which is taken to be a solution to the equation

\[(\nabla^2 + k^2)\psi_i(r, k) = 0\]

(3)

The scattered wave function \(\psi_s\) is given by

\[\psi_s(r, k) = g(r, k) \otimes_r V(r)\psi(r, k)\]

(4)

where \(\otimes_r\) denotes the convolution integral over all space \(r \in \mathbb{R}^3 \mapsto V(r)\) and \(g\) is the out-going free-space Green’s function

\[g(r, k) = -\frac{\exp(ikr)}{4\pi r},\ r \equiv |r|\]

which is the solution of

\[(\nabla^2 + k^2)g(r, k) = \delta^3(r)\]
On the basis of Equation (4) the scattering problem is ‘Given $V(r)$ evaluate $\psi_s(r, k)$’ and the inverse scattering problem is ‘Given $\psi_i(r, k)$ evaluate $V(r)$’. Both problems ideally require unconditional exact solutions. In this paper it is shown that exact solutions exist if $(\nabla^2 + k^2)V(r)\psi_i(r, k) = 0$. The proof of this result is the subject of the Section 4.

Note that if we could solve the equation

$$V(r)\psi(r, k) = W(r) \otimes_r \psi(r, k)$$

then Equation (4) becomes

$$\psi_s(r, k) = g(r, k) \otimes_r W(r) \otimes_r \psi(r, k)$$

and through application of the convolution theorem the scattering problem would be solved given that

$$\tilde{\psi}(u, k) = \tilde{\psi}_i(u, k) + \frac{\tilde{W}(u)\tilde{\psi}(u, k)}{u^2 - k^2 + i\epsilon}$$

where

$$\tilde{\psi}(u, k) = \int_{-\infty}^{\infty} \psi(r, k) \exp(-iu \cdot r)d^3r, \quad \tilde{W}(u) = \int_{-\infty}^{\infty} W(r) \exp(-iu \cdot r)d^3r$$

and it is noted that (for an arbitrarily small constant $\epsilon$ and the out-going Green’s function)

$$\tilde{g}(u, k) = \frac{-1}{u^2 - k^2 + i\epsilon}$$

4 Exact Solution

**Theorem 4.1** If and only if $(\nabla^2 + k^2)V(r)\psi_i = 0$ where $(\nabla^2 + k^2)\psi_i = 0$ then Equation (4) can be written in the form

$$\Psi(r, k) = g(r, k) \otimes_r V(r)\psi_i(r, k)$$

where (with $\leftrightarrow$ denoting Fourier transformation)

$$\Psi(r, k) \leftrightarrow \frac{\tilde{\psi}_i(u, k)\tilde{\psi}_s(u, k)}{\tilde{\psi}_i(u, k) + \tilde{\psi}_s(u, k)}$$

**Proof of Theorem 4.1** The key to the proof of this result is to write $V(r)\psi(r, k)$ as $W(r, k) \otimes_r \psi(r, k)$ where $W$ is some piecewise continuous auxiliary function. Thus we consider the equation

$$V(r)\psi(r, k) = W(r) \otimes_r \psi(r, k)$$

(5)
From Equation (1), and noting that

\[ \nabla^2[W(r) \otimes_r \psi(r, k)] = \nabla^2[W(r)] \otimes_r \psi(r, k) = W(r) \otimes_r \nabla^2\psi(r, k) \]

then

\[ \nabla^2[V(r)\psi(r, k)] = \nabla^2[W(r) \otimes_r \psi(r, k)] = W(r) \otimes_r \nabla^2\psi(r, k) \]

\[ = W(r) \otimes_r [V(r)\psi(r, k) - k^2\psi(r, k)] = W(r) \otimes_r [W(r) \otimes_r \psi(r, k) - k^2\psi(r, k)] \]

\[ = W(r) \otimes_r W(r) \otimes_r \psi(r, k) - k^2W(r) \otimes_r \psi(r, k) \]

Thus, introducing the function \( \phi(r, k) = W(r) \otimes_r \psi(r, k) \), Equation (1) can be written in the form (and without loss of generality)

\[ (\nabla^2 + k^2)\phi(r, k) = W(r, k) \otimes_r \phi(r, k) \]

But this equation has the fundamental solution

\[ \phi(r, k) = \phi_i(r, k) + g(r, k) \otimes_r W(r, k) \otimes_r \phi(r, k) \]

where \( \phi_i(r, k) \) is taken to be a solution to

\[ (\nabla^2 + k^2)\phi_i(r, k) = 0 \] (6)

Using the convolution theorem, we can write Equation (6) for \( \phi \) in \( u \)-space as

\[ \tilde{\phi}(u, k) = \tilde{\phi}_i(u, k) + \tilde{g}(u, k)\tilde{W}(u, k)\tilde{\phi}(u, k) \]

where \( \tilde{\phi}(u, k), \tilde{g}(u, k) \) and \( \tilde{W}(u, k) \) are the three-dimensional Fourier transforms of \( \phi(r, k), g(r, k) \) and \( W(r, k) \), respectively. Let \( \phi_i(r, k) = V(r)\psi_i(r, k) \) and let \( \tilde{V}(u) \) denote the Fourier transform of \( V(r) \). Writing this result in terms of \( \tilde{\psi}(u, k) \), application of the convolution and product theorems yields the \( u \)-space equation

\[ \frac{1}{(2\pi)^3} \tilde{V}(u, k) \otimes_u \tilde{\psi}_i(u, k) = \tilde{\psi}(u, k)\tilde{W}(u, k) - \tilde{g}(u, k)\tilde{\psi}(u, k)|\tilde{W}(u, k)|^2 \] (8)

However, given Equations (2) and (4) we can write

\[ \psi(r, k) = \psi_i(r, k) + g(r, k) \otimes_r V(r)\psi(r, k) \]

or, given Equation (5), and, using the convolution theorem

\[ \tilde{W}(u, k) = \frac{\tilde{\psi}(u, k) - \tilde{\psi}_i(u, k)}{\tilde{g}(u, k)\tilde{\psi}(u, k)} \]
Substituting this expression for \( \tilde{W}(u, k) \) into Equation (8) and noting that 
\( \tilde{\psi}(u, k) - \tilde{\psi}_i(u, k) = \tilde{\psi}_s(u, k) \) we obtain

\[
\frac{\tilde{\psi}_i(u, k)\tilde{\psi}_s(u, k)}{\tilde{\psi}_i(u, k) + \tilde{\psi}_s(u, k)} = \frac{1}{(2\pi)^3} \tilde{g}(u, k)[\tilde{V}(u, k) \otimes u \tilde{\psi}_i(u, k)]
\]

and taking inverse Fourier transforms we can write this result in the form

\[
\Psi(r, k) = g(r, k) \otimes_r V(r)\psi_i(r, k)
\]  

(9)

where

\[
\Psi(r, k) \leftrightarrow \frac{\tilde{\psi}_i(u, k)\tilde{\psi}_s(u, k)}{\tilde{\psi}_i(u, k) + \tilde{\psi}_s(u, k)}
\]

**Corollary 4.1** This proof is dependent on \( \phi_i(r, k) = V(r)\psi_i(r, k) \) satisfying Equation (7) given that \( \psi_i(r, k) \) satisfies Equation (3) and implies that \( V(r) \) satisfies the equation

\[
\nabla^2 V(r) + 2\nabla V(r) \cdot \nabla \ln \psi_i(r, k) = 0
\]

(10)

Thus for any phase only function \( \psi_i(r, k) \) with phase function \( \phi(r, k) \), say,

\[
\nabla^2 V(r) + 2i\nabla V(r) \cdot \nabla \phi(r, k) = 0
\]

and hence for any real scattering potential \( V(r) \) such that \( \text{Im}V(r) = 0 \), Equation (10) implies that \( V(r) \) satisfy Laplace’s equation \( \nabla^2 V(r) = 0 \).

**Corollary 4.2** For \( \psi_i(r, k) = \exp(ik\hat{n}_i \cdot r) \) (where \( \hat{n}_i \) is a unit vector pointing in the direction of the incident wave function), in the far-field Equation (9) can be written in the form

\[
\frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{\tilde{\psi}_i(u, k)\tilde{\psi}_s(u, k)}{\psi_i(u, k) + \psi_s(u, k)} \exp(iku \cdot \cdot r) \, du = -\frac{\exp(ikr)}{4\pi r} \int_{\mathbb{R}^3} V(r') \exp(-ik\hat{N} \cdot r') \, dr', \quad r \to \infty
\]

(11)

where, from Equation (10), \( V(r) \) satisfies the equation

\[
\nabla^2 V(r) + 2ik\hat{n}_i \cdot \nabla V(r) = 0
\]

and \( \hat{N} = \hat{n}_s - \hat{n}_i \) where \( \hat{n}_s \) is the unit vector pointing in the direction of the scattered field and we note that \( |\hat{N}| = 2\sin^2(\theta/2) \) where \( \theta = \cos^{-1}(\hat{n}_i \cdot \hat{n}_s) \) is the scattering angle.
Let
\[ \psi_s(r, k) = -\frac{\exp(ikr)}{4\pi r} A_s(k\hat{N}), \ r \to \infty \]
where \( A_s(k\hat{N}) \) is the scattering amplitude in the far-field. Then, using the Shift Theorem, and, working with spherical polar coordinates,
\[
\tilde{\psi}_s(u, k) = -A_s(k\hat{N}) \int_{\mathbb{R}^3} \frac{\exp(ikr)}{4\pi r} \exp(-iu \cdot r) d^3r
\]
\[
= -A_s(k\hat{N}) \int_{\mathbb{R}^3} \frac{\exp[ik(r + a)]}{4\pi(r + a)} \exp(-iu \cdot r) d^3r, \ a \to \infty
\]
\[
= -A_s(k\hat{N}) \frac{\exp(ika)}{4\pi a} \int_{\mathbb{R}^3} \frac{\exp(ikr)}{4\pi r} \exp(-iu \cdot r) d^3r
\]
\[
= -A_s(k\hat{N}) \frac{\exp(ika)}{a} \int_0^R \text{sinc}(ur) \exp(ikr) r^2 dr,
\]
where \( R \) is the radius of the effective range of the scattering potential and
\[
\tilde{\psi}_i(u, k) = \int_{\mathbb{R}^3} \exp(ik\hat{n}_i \cdot r) \exp(-iu \cdot r) d^3r
\]
\[
= \int_{\mathbb{R}^3} \exp[ik\hat{n}_i \cdot (r + a)] \exp(-iu \cdot r) d^3r, \ |a| \to \infty
\]
\[
= \exp(ik\hat{n}_i \cdot a) \int_{\mathbb{R}^3} \exp(ik\hat{n}_i \cdot r) \exp(-iu \cdot r) d^3r
\]
\[
= \exp(ik\hat{n}_i \cdot a) \int_0^R \text{sinc}(u |r - k\hat{n}_i|) r^2 dr
\]
Noting that
\[
\int_{\mathbb{R}^3} \frac{\exp(ikr)}{4\pi r} \exp(-iu \cdot r) d^3r \int_{\mathbb{R}^3} V(r') \exp(-ik\hat{N} \cdot r') d^3r'
\]
\[
= \frac{\exp(ika)}{a} \int_0^R \text{sinc}(ur) \exp(ikr) r^2 dr \tilde{V}(k\hat{N})
\]
where
\[
\tilde{V}(k\hat{N}) \equiv \int_{\mathbb{R}^3} V(r') \exp(-ik\hat{N} \cdot r') d^3r'
\]
Equation (11) can be written in the form
\[
\frac{A_s(k\hat{N})}{1 + cA_s(k\hat{N})} = \tilde{V}(k\hat{N}), \quad c = \frac{\exp(ika) \int_0^R \text{sinc}(ur) \exp(ikr)r^2dr}{a \exp(ikn_i \cdot a) \int_0^R \text{sinc}(|u - k\hat{n}_i| r)r^2dr}
\]

\[
= \frac{1}{a} \exp[ika(1 - \cos \chi)], \quad \cos \chi = \frac{\hat{n}_i \cdot \frac{a}{|a|}}{\text{as } R \to 0}
\]

and thus, for \( \chi \sim 0 \)

\[
\tilde{V}(k\hat{N}) = \frac{A_s(k\hat{N})}{1 + A_s(k\hat{N})/a} \quad \text{and} \quad A_s(k\hat{N}) = \frac{\tilde{V}(k\hat{N})}{1 - \tilde{V}(k\hat{N})/a}
\]

**Corollary 4.3** For \( r \in \mathbb{R}^1 \mapsto V(x) \), consider the reflection coefficient

\[
R(k) = \int_{-\infty}^{\infty} V(x) \exp(-2ikx) dx
\]

(i.e. the back scattered field when \( \hat{n}_s = -\hat{n}_i \)) given that the out-going free-space Green's function for \( r \in \mathbb{R}^1 \) is

\[
g(x, k) = -\frac{i}{2k} \exp(ikx)
\]

For \( |x| \to 0 \) Equation (11) is given by

\[
\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\tilde{\psi}_i(u, k)\tilde{\psi}_s(u, k)}{\tilde{\psi}_i(u, k) + \tilde{\psi}_s(u, k)} \exp(ixu) du = -\exp(ikx) \frac{1}{2ik} \tilde{V}(2k)
\]

where

\[
\tilde{V}(2k) = \int_{x' \in \mathbb{R}^1} V(x') \exp(-2ikx') dx'
\]

and for reflection amplitude \( r(k), \psi_s(x, k) = \exp(ikx)r(k), \quad |x| \to \infty \) given incident unit wave function \( \psi_i(x, k) = \exp(-ikx) \). Let \( V(x') \forall x' \in [-X/2, X/2] \), then using the same method as exercised in Corollary 4.2, and, noting that

\[
\int_{x \notin \mathbb{R}^1} \psi_s(x, k) \exp(-ixu) dx \int_{x' \in \mathbb{R}^1} \psi_s(x + a, k) \exp(-ixu) dx, \quad a \to \infty
\]

\[
= \exp(ika) X \text{sinc}[(u - k)X/2]
\]
and that
\[
\frac{\text{sinc}[(u - k)X/2]}{\text{sinc}[(u + k)X/2]} = 1
\]
we obtain
\[
\frac{r(k)}{1 + \exp(2ika)r(k)} = -\frac{\tilde{V}(2k)}{2ik}
\]
Thus using the convolution theorem, we have
\[
R(x) + K(x) + \delta(x + 2a) \otimes_x R(x) \otimes_x K(x) = 0
\]
where
\[
R(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} r(k) \exp(ikx) dk, \quad V(x) = 2\frac{d}{dx} K(2x)
\]
and \(\otimes_x\) denotes the convolution along the line \(x \in (-\infty, \infty)\). However, noting that
\[
\delta(x + 2a) \otimes_x R(x) \otimes_x K(x) = R(x) \otimes_x K(x + 2a)
\]
and that (with \(\dagger\) denoting Fourier transformation)
\[
V(x + 2a) = 2\frac{d}{dx} K(2x + 4a)
\]
\[
\dagger
\]
\[
\exp(2ika)\tilde{V}(k) = \exp(2ika)\frac{1}{2}\tilde{K}(k/2)
\]
\[
\dagger
\]
\[
V(x) = 2\frac{d}{dx} K(2x)
\]
we can write
\[
R(x) + K(x) + R(x) \otimes_x K(x) = 0
\]
Equation (12) is the Gel’fand-Levitan equation (e.g. [11], [12] and [13]).

**Remark 4.1** The Corollary 4.1 sets out a condition that is based on letting \(\phi_i = V\psi_i\) where \(\psi_i\) is a solution to \((\nabla^2 + k^2)\psi_i = 0\). However, another implication of the equation \((\nabla^2 + k^2)V\psi = 0\) is that
\[
(\nabla^2 + k^2)(\nabla^2 + k^2)\psi(r, k) = (\nabla^2 + k^2)(\nabla^2 + k^2)\psi_s(r, k)
\]
\[
= (\nabla^4 + 2k^2\nabla^2 + k^4)\psi_s(r, k) = 0
\]
given that \((\nabla^2 + k^2)\psi_i = 0\). This result is entirely self consistent with the equation \((\nabla^2 + k^2)V\psi = 0\) as can be shown through substitution of \(\psi_s = g \otimes_r V\psi\).
Remark 4.2 Equation (9) reduces the scattering wave function under the Born approximation when
\[
\frac{\tilde{\psi}_i(u, k)\tilde{\psi}_s(u, k)}{\tilde{\psi}_i(u, k) + \tilde{\psi}_s(u, k)} = \tilde{\psi}_s(u, k) \left[ 1 + \frac{\tilde{\psi}_s(u, k)}{\tilde{\psi}_i(u, k)} \right] \sim \tilde{\psi}_s(u, k)
\]
and
\[
\psi_s(r, k) = g(r, k) \otimes_r V(r)\psi_i(r, k)
\]

5 Solution for Orthonormal Functions \(\psi_i(r, k)\)

Theorem 5.1 If
\[
\psi_i^*(r, k) \otimes_r \psi_i(r, k) = \delta^3(r)
\]
then Equation (3) is satisfied and the scattered field is given by the series solution
\[
\psi_s(r, k) = g(r, k) \otimes_r V(r)\psi_i(r, k)
\]
\[
+ [g(r, k) \otimes_r V(r)\psi_i(r, k)] \otimes_r [\psi_i^*(r, k) \otimes_r g(r, k) \otimes_r V(r)\psi_i(r, k)] + \ldots \quad (13)
\]

Proof of Theorem 5.1 Equation (3) is satisfied since
\[
\psi_i^*(r, k) \otimes_r (\nabla^2 + k^2)\psi_i(r, k) = \psi_i^*(r, k) \otimes_r (-k^2 + k^2)\psi_i(r, k)
\]
\[
= (-k^2 + k^2)\psi_i^*(r, k) \otimes_r \psi_i(r, k) = (k^2 - k^2)\delta^3(r) = 0
\]
From Equation (9) we can write
\[
\psi_i(r, k) \otimes_r \psi_s(r, k) = \psi_i(r, k) \otimes_r [g(r, k) \otimes_r V(r)\psi_i(r, k)]
\]
\[
+ \psi_s(r, k) \otimes_r [g(r, k) \otimes_r V(r)\psi_i(r, k)]
\]
Convolving each term of this equation with \(\psi_i^*(r, k)\) we then have
\[
\psi_s(r, k) = [g(r, k) \otimes_r V(r)\psi_i(r, k)] + \psi_i^*(r, k) \otimes_r \psi_s(r, k) \otimes_r [g(r, k) \otimes_r V(r)\psi_i(r, k)]
\]
so that upon Fourier transforming and rearranging,
\[
\tilde{\psi}_s(u, k) = \frac{1}{(2\pi)^3} \tilde{g}(u, k)\tilde{V}(u) \otimes_u \tilde{\psi}_i(u, k)
\]
\[
\times \left[ 1 - \frac{1}{(2\pi)^3} \tilde{\psi}_i^*(u, k)\tilde{g}(u, k)\tilde{V}(u) \otimes_u \tilde{\psi}_i(u, k) \right]^{-1}
\]
\[
= \frac{1}{(2\pi)^3} \tilde{g}(u, k)\tilde{V}(u) \otimes_u \tilde{\psi}_i(u, k)
\]
\[
+ \left[ \frac{1}{(2\pi)^3} \tilde{g}(u, k) \tilde{V}(u) \otimes_u \widetilde{\psi}_1(u, k) \right] \left[ \frac{1}{(2\pi)^3} \tilde{\psi}_1^*(u, k) \tilde{g}(u, k) \tilde{V}(u) \otimes_u \widetilde{\psi}_1(u, k) \right] + \ldots
\]
given that
\[
\left| \frac{1}{(2\pi)^3} \tilde{\psi}_1^*(u, k) \tilde{g}(u, k) \tilde{V}(u) \otimes_u \widetilde{\psi}_1(u, k) \right| < 1 \tag{14}
\]
Inverse Fourier transformation then yields Equation (13).

**Corollary 5.1** This result relies on the orthonormality condition
\[
\psi_i^*(r, k) \otimes_r \psi_i(r, k) = \delta^3(r)
\]
and Condition (14) to develop the series solution given. For an orthonormal function \( \psi_i \) Condition (14) places a limit of the amplitude spectrum of the scattering potential. With regard to the class of orthonormal spectrum available, one such function is \( \exp(i\alpha r^2) \) where \( \alpha \) is a constant since in this case

\[
\exp(-i\alpha r^2) \otimes_r \exp(i\alpha r^2) = \int_{-\infty}^{\infty} \exp[-i\alpha |r - s|^2] \exp(i\alpha s^2) d^3s
\]

\[
= \int_{-\infty}^{\infty} \exp(-i\alpha^2) \exp(2i\alpha r \cdot s) d^3s = (2\pi)^3 \exp(-i\alpha^2) \delta^3(2\alpha r)
\]

\[
= (4\pi |\alpha|)^3 \exp(-i\alpha^2) \delta^3(r)
\]

### 6 Conclusions

The primary purpose of this paper is to introduce Theorem 4.1 which provides an exact and self-consistent scattering solution based on Equation (9) conditional upon Equation (7). It is noted that from Equation (9) an exact inverse solution may be developed. A series solution for the scattered field is available based on Theorem 5.1 which is predicated on the incident wave function being an orthonormal function.

### References


Received: April, 2015