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WEAK GRADIENT INVERSE SCHRÖDINGER SCATTERING

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ABSTRACT. The paper briefly reviews formal methods and associated conditions for solving the forward and inverse Schrödinger scattering problem for a three-dimensional elastic scattering potential. These methods are based on an application of the Green's function and are conditional upon the properties of the scattering potential, e.g. that the scattering potential is a 'weak scatterer'. In this paper, we explore an alternative route to solving the problem which depends on properties imposed on the scattered wavefield rather than the scattering potential. In particular, we explore the case when the gradient of the scattered wavefield is weak relative to its frequency. An inverse scattering solution is then derived from which iterative forward scattering solutions can be formulated. The properties of this solution are studied including various simplifications that can be made and the conditions upon which they rely. This includes a phase only condition that is used to compute the Rutherford scattering cross-section with a second order correction. Finally, it is shown how the approach can be applied to the relativistic case when the scattering problem is determined by the Klein-Gordon equation and for electromagnetic scattering problems that are based on the inhomogeneous Helmholtz equation.

1. INTRODUCTION

The scattering of an incident wave from an elastic scattering potential V is determined by the general solution of the three-dimensional Schrödinger equation [1], [2]

$$(\nabla^2 + k^2)\psi(\mathbf{r}, k) = V(\mathbf{r})\psi(\mathbf{r}, k), \quad \mathbf{r} \in \mathbb{R}^3 \tag{1}$$

where k is the wavenumber and ψ is a complex wavefunction. The incident wavefunction, which is taken to describe a unit plane wave ψ_i, is assumed to have a narrow-band spectrum so that k is, effectively, a constant.

Equation (1) is derived from the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) = \frac{-\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}, t) + V(\mathbf{r})\Psi(\mathbf{r}, t) \tag{2}$$

where m is the mass of a particle described wavefunction Ψ. This is the non-relativistic 'energy equation' $E = V + \mid \mathbf{p} \mid^2 /(2m)$ for potential energy V with energy E and momentum $\mathbf{p}$ operators $E \rightarrow i\hbar\partial_t$ and $\mathbf{p} \rightarrow -i\hbar\nabla$, respectively, where $h = 2\pi\hbar$ is Planck's constant. For $\Psi(\mathbf{r}, t) = \psi(\mathbf{r}, \omega)\exp(-i\omega t)$ and with $k^2 = 2m\omega/\hbar = 2mE/\hbar^2$ and $V := 2mV/\hbar^2$, the time-independent version of equation (2) given by equation (1) is obtained.

THE POROBLEM. We require a solution to equation (1) for the scattered wavefunction ψ_s from which the 'scattering cross-section' given by $\mid \psi_s \mid^2$ can be evaluated.

Let $\psi = \psi_i^{\pm} + \psi_s$ where $\psi_i^{\pm}$ is the solution of

$$(\nabla^2 + k^2)\psi_i^{\pm}(\mathbf{r}, k) = 0 \tag{3}$$

Then, $\psi_i^{\pm} = \exp(\pm ik\hat{\mathbf{n}}_i \cdot \mathbf{r})$ where $\hat{\mathbf{n}}_i$ is a unit vector that points in the direction of the incident plane wave with unit amplitude.

For the condition

$$V(\mathbf{r}) \to 0 \;\text{ as }\; r \equiv\mid \mathbf{r} \mid\to \infty \tag{4}$$

the Green's function transformation of equation (1) yields the Lippmann-Schwinger equation [3]

$$\psi(\mathbf{r}, k) = \psi_i^{\pm}(\mathbf{r}, k) + \psi_s(\mathbf{r}, k) \tag{5}$$

where

$$\psi_s(\mathbf{r}, k) = g(r, k) \circ V(\mathbf{r})\psi(\mathbf{r}, k) \;\text{ and }\; g(r, k) = -\frac{\exp(ikr)}{4\pi r} \tag{6}$$

is the 'out-going' free space Green's function which is the solution of

$$(\nabla^2 + k^2)g(r, k) = \delta^3(\mathbf{r}) \tag{7}$$

The symbol $\circ$ denotes the three-dimensional convolution integral, i.e. for two piecewise continuous functions $f_1(\mathbf{r})$ and $f_2(\mathbf{r})$,

$$f_1(\mathbf{r}) \circ f_2(\mathbf{r}) \equiv \int\limits_{R^3} f_1(\mathbf{r} - \mathbf{s})f_2(\mathbf{s})d^3\mathbf{s} \tag{8}$$

and

$$f_1(r) \circ f_2(\mathbf{r}) \equiv \int\limits_{R^3} f_1(\mid \mathbf{r} - \mathbf{s} \mid)f_2(\mathbf{s})d^3\mathbf{s} \tag{9}$$

Formally, equation (5) requires that

$$\psi(\mathbf{r}, k) \to 0 \;\text{ and }\; \nabla\psi(\mathbf{r}, k) \to 0 \;\text{ as }\; r \to \infty \tag{10}$$

so that, by Green's theorem (where $\mathcal{S}$ is the surface associated with spatial domain $\mathcal{D}$),

$$\int\limits_{\mathcal{D}} \nabla \cdot (g\nabla\psi - \psi\nabla g)d^3\mathbf{r} = \oint\limits_{\mathcal{S}} (g\nabla\psi - \psi\nabla g) \cdot \hat{\mathbf{n}}d^2\mathbf{r} = 0 \tag{11}$$

given that the scattering potential is not of compact support by condition (4) but in the infinite domain with a surface at infinity.

Equation (6) allows us to define the forward and inverse scattering problems as follows:

Forward Scattering Problem:	*Given* V *calculate* ψ_s
Inverse Scattering Problem:	*Given* ψ_s *calculate* V

We note that equation (5) is the fundamental basis for the Schrödinger (elastic) scattering problem but that if condition (4) holds, the problems defined above can be stated in terms of equation (1). In other words, under condition (4), Equations (1) and (5) define the same problem since it is clear that

$$\begin{aligned}(\nabla^2 + k^2)\psi(\mathbf{r}, k) &= (\nabla^2 + k^2)\psi_i^{\pm}(\mathbf{r}, k) + (\nabla^2 + k^2)[g(r, k) \circ V(\mathbf{r})\psi(\mathbf{r}, k)] \\ &= \delta^3(\mathbf{r}) \circ V(\mathbf{r})\psi(\mathbf{r}, k) = V(\mathbf{r})\psi(\mathbf{r}, k)\end{aligned} \tag{12}$$

2. Formal Scattering and Inverse Scattering Solutions

Given equation (6), a solution for ψ_s can be obtained by iteration to give the (Born) series solution

$$\psi_s(\mathbf{r}, k) = g(r, k)\circ V(\mathbf{r})\psi_i^{\pm}(\mathbf{r}, k) + g(r, k)\circ V(\mathbf{r})[g(r)\circ V(\mathbf{r})\psi_i^{\pm}(\mathbf{r}, k)] + ... \tag{13}$$

Each term in equation (13) expresses higher order scattering effects which 'reflects' their causal nature, i.e. a $(n + 1)^{\text{th}}$-order scattering effect can not occur before n^{th}-order scattering has taken place.

LEMMA 2.1 Equation (5) converges under the condition

$$\| g(r, k) \circ V(\mathbf{r})\|_2 < 1 \tag{14}$$

where $\| \bullet \|_2$ denotes the (Euclidean) norm in $L^2(\mathbb{R}^3; d^3\mathbf{r})$.
Proof. Consider an iterative solution to Equation (5) of the form

$$\psi_{n+1}(\mathbf{r}, k) = \psi_i^{\pm}(\mathbf{r}, k) + \hat{I}V(\mathbf{r})\psi_n(\mathbf{r}, k) \tag{15}$$

where

$$\psi_0(\mathbf{r}, k) \equiv \psi_i^{\pm}(\mathbf{r}, k) \tag{16}$$

and $\hat{I}$ is the convolution integral operator

$$\hat{I} = g(r, k)\circ \tag{17}$$

For each iteration n, consider the solution to be given by $\psi_n = \psi + \epsilon_n$ where ϵ_n is the error associated with the solution at iteration n and ψ is the exact solution. A sufficient condition for convergence is that $\epsilon_n \to 0$ as $n \to \infty$ and since

$$\psi + \epsilon_{n+1} = \psi_i^{\pm} + \hat{I}[V(\psi + \epsilon_n)] = \psi_i^{\pm} + \hat{I}(V\psi) + \hat{I}(V\epsilon_n) \tag{18}$$

we have

$$\epsilon_{n+1} = \hat{I}(V\epsilon_n) \tag{19}$$

since $\psi = \psi_i^{\pm} + \hat{I}(V\psi)$. Thus,

$$\epsilon_n = \hat{I}V[\hat{I}V(\hat{I}V...\epsilon_0)] \tag{20}$$

from which it follows that

$$\|\epsilon_n\|_2 \leq \|\hat{I}V\|_2^n \|\epsilon_0\|_2 \tag{21}$$

The condition for convergence therefore becomes

$$\lim_{n\to\infty} \frac{\|\epsilon_n\|_2}{\|\epsilon_0\|_2} \leq \lim_{n\to\infty} \|\hat{I}V\|_2^n = 0, \quad \Longrightarrow \|\hat{I}V\|_2 < 1 \tag{22}$$

COROLLARY 2.1. Under the condition

$$\|g(r,k) \circ V(\mathbf{r})\|_2 << 1, \tag{23}$$

$$\psi_s(\mathbf{r},k) = g(r,k) \circ V(\mathbf{r})\psi_i^{\pm}(\mathbf{r},k) \tag{24}$$

which is the first iterate corresponding to the first term of equation (13).

REMARK 2.1. Equation (24) is an expression for the scattered wavefunction under the weak scattering condition - the Born approximation - which is equivalent to assuming that $\|\psi_s\|_2 << \|\psi_i^{\pm}\|_2$ in equation (6). Similarly, the convergence criterion associated with equation (13), i.e. $\|\hat{I}V\|_2 < 1$, is equivalent to assuming that $\|\psi_s\|_2 < \|\psi_i^{\pm}\|_2$ in equation (6)

REMARK 2.2. If $V(\mathbf{r})$ is of compact support so that $V(\mathbf{r})$ exists $\forall \mathbf{r} \in \mathcal{D}$ and is additionally a sphere with radius R, then, since

$$\|g(r,k) \circ V(\mathbf{r})\|_2 \leq \|g(r,k)\|_2 \; \|V(\mathbf{r})\|_2, \tag{25}$$

(26)

$$\|g(r,k) \circ V(\mathbf{r})\|_2 \leq \frac{1}{\sqrt{3}} R^2 \langle V(\mathbf{r})\rangle \quad \text{where} \quad \langle V(\mathbf{r})\rangle = \sqrt{\frac{\int\limits_{\mathbf{r}\in\mathcal{D}} \mid V(\mathbf{r}) \mid^2 d^3\mathbf{r}}{\int\limits_{\mathbf{r}\in\mathcal{D}} d^3\mathbf{r}}}$$

and condition (23) becomes $\langle V(\mathbf{r})\rangle << R^{-2}$.

REMARK 2.3 Equation (24) is an exact solution to the equation

$$V = (\psi_i^{\pm})^{-1}(\nabla^2 + k^2)\psi_s \tag{27}$$

since

$$\begin{aligned}(\nabla^2 + k^2)\psi_s(\mathbf{r}, k) &= (\nabla^2 + k^2)g(r, k) \circ [V(\mathbf{r})\psi_i^{\pm}(\mathbf{r}, k)] \\ &= \delta^3(\mathbf{r}) \circ V(\mathbf{r})\psi_i^{\pm}(\mathbf{r}, k) = V(\mathbf{r})\psi_i^{\pm}(\mathbf{r}, k)\end{aligned} \tag{28}$$

LEMMA 2.2. Let $\psi_s(\mathbf{r}, k) = g(r, k) \circ V(\mathbf{r})\psi_i^{+}(\mathbf{r}, k)$, then

$$\psi_s(\mathbf{r}_s, k) = \frac{\exp(ikr_s)}{4\pi r_s}\widetilde{V}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)], \quad r_s \to \infty \tag{29}$$

where

$$\widetilde{V}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = \int_{R^3} V(\mathbf{r})\exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)\cdot\mathbf{r}]d^3\mathbf{r}, \quad \hat{\mathbf{n}}_s = \mathbf{r}_s/r_s \tag{30}$$

and $\mathbf{r}_s$ is the vector position at which the scattered field ψ_s is detected.
Proof.

$$|\, \mathbf{r}_s - \mathbf{r} \,| = r_s\left(1 - \frac{\mathbf{r}\cdot\mathbf{r}_s}{r_s^2} + \frac{r^2}{2r_s^2} + ...\right) = r_s - \mathbf{r}\cdot\hat{\mathbf{n}}_s, \quad r_s \to \infty \tag{31}$$

so that

$$g(|\, \mathbf{r}_s - \mathbf{r} \,|, k) = \frac{\exp(ikr_s)}{4\pi r_s}\exp(-ik\hat{\mathbf{n}}_s\cdot\mathbf{r}), \quad r_s \to \infty \tag{32}$$

and, for ψ_i^{+}, equation (24) transforms to

$$\psi_s(\mathbf{r}_s, k) = \frac{\exp(ikr_s)}{4\pi r_s}\int_{R^3} V(\mathbf{r})\exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)\cdot\mathbf{r}]d^3\mathbf{r}, \quad r_s \to \infty \tag{33}$$

REMARK 2.4. Equation (33) shows that the forward scattering and inverse scattering problems are reduced to forward Fourier and inverse Fourier transformations respectively, i.e. for $\|g(r, k) \circ V(\mathbf{r})\|_2 << 1$, analysis of the solution in the far-field (i.e. when $r_s \to \infty$) is equivalent to Fourier space analysis.

REMARK 2.5. The function $\exp[ikr_s/(4\pi r_s)]$ in equation (33) is a complex scaling constant and we may therefore define the 'scattering amplitude' as

$$A[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = \int_{R^3} V(\mathbf{r})\exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)\cdot\mathbf{r}]d^3\mathbf{r} \tag{34}$$

This Fourier transform relationship between the scattering potential V and the scattering amplitude A is fundamental to Schrödinger scattering applications such as ion beam analysis [4], [5], for example, but implicitly relies on condition (23).

REMARK 2.6. Strictly speaking, we should define the scattering amplitude in terms of the integral

$$A[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = \int\limits_{\mathbf{r}\in\mathcal{D}} V(\mathbf{r}) \exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i) \cdot \mathbf{r}] d^3\mathbf{r} \tag{35}$$

This is because the Fourier transform is obtained via the argument that $r/r_s \rightarrow 0$ as $r_s \rightarrow \infty$ $\forall r$ which is inconsistent if $r \in [0, \infty)$. However, if we do define the Fourier integral for $\mathbf{r} \in \mathcal{D}$ to make this argument strictly consistent, then the surface integral given in equation (11), should, strictly speaking, be taken to be non-zero. Instead, we consider the scattering amplitude to be defined in terms of equation (35) on the understanding that the contribution of this surface integral is negligible. This 'balancing act' allows us to formally define the inverse scattering solution to be given by

$$V(\mathbf{r}) = \frac{1}{(2\pi)^3} \int\limits_{R^3} A[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \exp[ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i) \cdot \mathbf{r}] d^3[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \tag{36}$$

under the conditions that: (i) $\|\psi_s\|_2 << \|\psi_i\|_2$; (ii) $r_s \rightarrow \infty$

LAMMA 2.3. An inverse solution to equation (5) is

$$V(\mathbf{r}) = \sum_{n=1}^{\infty} V_n(\mathbf{r}), \tag{37}$$

$$V_1 = \hat{J}\psi_s, \quad V_2 = \hat{J}[\hat{I}V_1(\hat{I}V_1\psi_i^{\pm})], \quad ... \tag{38}$$

where $\hat{J}$ is an operator such that

$$\hat{J}(\hat{I}V_n\psi_i) = V_n \tag{39}$$

Proof. (Jost-Kohn [6])

Let

$$V = \sum_{n=1}^{\infty} \epsilon^n V_n \quad \text{and} \quad \epsilon\psi_s := \psi - \psi_i^{\pm} \tag{40}$$

Substitution of these equations into equation (13) gives

$$\epsilon\psi_s = \hat{I}(\epsilon V_1 + \epsilon^2 V_2 + \epsilon^3 V_3 + ...)\psi_i^{\pm} \tag{41}$$

$$+\hat{I}(\epsilon V_1 + \epsilon^2 V_2 + \epsilon^3 V_3 + ...)[\hat{I}(\epsilon V_1 + \epsilon^2 V_2 + \epsilon^3 V_3 + ...)\psi_i^{\pm}] + ...$$

Equating terms with common coefficients $\epsilon, \epsilon^2, ...$ we have

For $n = 1$:

$$\psi_s = \hat{I} V_1 \psi_i^{\pm}, \Rightarrow V_1 = \hat{J}\psi_s \tag{42}$$

For $n = 2$:

$$0 = \hat{I} V_2 \psi_i^{\pm} + \hat{I} V_1 (\hat{I} V_1 \psi_i), \Rightarrow V_2 = -\hat{J}[\hat{I} V_1 (\hat{I} V_1 \psi_i^{\pm}) \tag{43}$$

and so on for $n = 3, 4, ...$ Evaluating V_n for $n = 1, 2, ..., \infty$, $V(\mathbf{r})$ is obtained from equation (37) with $\epsilon = 1$.

REMARK 2.7. This iterative inverse solution is not unconditional; it requires convergence of the series solution to the forward scattering problem - equation (13)

REMARK 2.8. For $n = 1$, the formal inverse solution is given by equation (36) for $r_s \to \infty$.

DISCUSSION. This section has assembled the principal results associated with formal solutions to the forward and inverse scattering problems [7]. The following points are noted: (i) All the results presented are based on the Green's function transformation of equation (1); (ii) both forward and inverse scattering solutions are based on iterative series solutions. In the latter case, an iterative (inverse scattering) solution is formulated to an iterative (forward scattering) solution. Consequently many practical applications associated with inverse scattering solutions only utilize equation (35) under condition (23). In the following section, we consider a conditional approach to this problem that avoids using a Green's function transformation and is based a weak gradient condition.

3. Green's Function Independent Solutions

Under condition (4), Equations (1) and (5) are entirely inter-operable. This property underlies an approach that is based on developing an inverse solution for V given ψ based on equation (1) avoiding the use of a Green's function transformation.

THEOREM 3.1. Given equations (1) and (5) and under condition (4),

$$V(\mathbf{r}) = \frac{\psi^*(\mathbf{r},k)}{\mid \psi(\mathbf{r},k) \mid^2}\nabla^2\left[\frac{k^2}{4\pi r}\circ\psi_s(\mathbf{r},k)+\psi_s(\mathbf{r},k)\right] \tag{44}$$

Proof. From equation (5), we can write

$$(\psi - \psi_i^{\pm}) = g\circ V\psi \tag{45}$$

Let q be a piecewise continuous auxiliary function such that

$$q\circ(\psi - \psi_i^{\pm}) = q\circ(g\circ V\psi) \tag{46}$$

Taking the Laplacian operator of this equation,

$$\nabla^2[q\circ(\psi-\psi_i^{\pm})] = \nabla^2(q\circ g\circ V\psi) = \nabla^2(q\circ g)\circ V\psi = V\psi \tag{47}$$

provided

$$\nabla^2(q\circ g) = \delta^3 \tag{48}$$

But

$$\nabla^2(q\circ g) = q\circ\nabla^2 g = q\circ(-k^2 g+\delta^3) = -k^2 q\circ g + q \tag{49}$$

and hence

$$q = \delta^3 + k^2 q\circ g \tag{50}$$

so that

$$\begin{aligned}\nabla^2[q\circ(\psi-\psi_i^{\pm})] &= \nabla^2[\delta^3\circ(\psi-\psi_i^{\pm}) + k^2 q\circ g\circ(\psi-\psi_i^{\pm})] \\ &= \nabla^2[(\psi-\psi_i^{\pm}) + k^2 q\circ g\circ(\psi-\psi_i^{\pm})] = V\psi\end{aligned} \tag{51}$$

Thus,

$$V = \frac{1}{\psi}\nabla^2\left[k^2 q\circ g\circ(\psi-\psi_i^{\pm}) + (\psi-\psi_i^{\pm})\right] \tag{52}$$

where q is determined by the solution of

$$\nabla^2(q\circ g) = \delta^3 \tag{53}$$

given by

$$q\circ g = -\frac{1}{4\pi r} \tag{54}$$

so that

$$V = \frac{1}{\psi}\nabla^2\left[(\psi-\psi_i^{\pm})) - \frac{k^2}{4\pi r}\circ(\psi-\psi_i^{\pm})\right] \tag{55}$$

Finally, since $\psi = \psi_i^{\pm} + \psi_s$, we can write

$$V = \frac{1}{\psi}\nabla^2\left[\psi_s - \frac{k^2}{4\pi r}\circ\psi_s\right] = \frac{\psi^*}{\mid\psi\mid^2}\nabla^2\left[\psi_s - \frac{k^2}{4\pi r}\circ\psi_s\right] \tag{56}$$

This proof requires that the auxiliary function q exists, i.e. that there exists a solution to equation (54). A general solution for q is therefore provided in the following Theorem.

THEOREM 3.2. Given equation (54), the solution for q is

$$q = \delta^3 - \frac{k^2}{4\pi r} \tag{57}$$

Proof. Taking the Laplacian of equation (54), we have

$$g \circ \nabla^2 q = \delta^3 \tag{58}$$

Taking the Fourier transform of equation (58), we obtain

$$\frac{u^2}{u^2 - k^2} Q(\mathbf{u}) = 1 \tag{59}$$

where

$$Q(\mathbf{u}) = \int_{R^3} q(\mathbf{r}) \exp(-i\mathbf{u} \cdot \mathbf{r}) d^3\mathbf{r} \tag{60}$$

Thus, using spherical polar coordinates,

$$\begin{aligned}
q(\mathbf{r}) &= \frac{1}{(2\pi)^3} \int_{R^3} \left(1 - \frac{k^2}{u^2}\right) \exp(i\mathbf{u} \cdot \mathbf{r}) d^3\mathbf{u} \\
&= \delta^3 - \frac{k^2}{(2\pi)^3} \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) \int_0^{\infty} du \exp(iur\cos\theta) \\
&= \delta^3 - \frac{k^2}{2\pi^2 r} \int_0^{\infty} \frac{\sin(ur)}{u} du \\
&= \delta^3 - \frac{k^2}{4\pi r}, \quad \int_0^{\infty} \frac{\sin x}{x} dx = \frac{\pi}{2} \qquad (61)
\end{aligned}$$

COROLLARY 3.1. Since

$$(\nabla^2 + k^2)\psi_i^{\pm} = 0 \tag{62}$$

and noting that

$$\nabla^2 \left(\frac{1}{4\pi r}\right) = -\delta^3(r) \tag{63}$$

it follows that

$$\begin{aligned} V &= \frac{1}{\psi}\nabla^2\left[(\psi-\psi_i^{\pm}) - \frac{k^2}{4\pi r}\circ(\psi-\psi_i^{\pm})\right] \\ &= \frac{1}{\psi}\left[k^2\delta^3\circ(\psi-\psi_i^{\pm}) + (\nabla^2\psi - \nabla^2\psi_i^{\pm})\right] \\ &= \frac{1}{\psi}\left[k^2(\psi-\psi_i^{\pm}) + \nabla^2\psi + \nabla^2\psi_i^{\pm}\right] \\ &= \frac{1}{\psi}\left[(\nabla^2\psi + k^2\psi) + \nabla^2\psi_i^{\pm} + k^2\psi_i^{\pm}\right] \\ &= \frac{1}{\psi}(\nabla^2 + k^2)\psi \end{aligned} \tag{64}$$

which recovers the Schrödinger equation - equation (1).

3.1. **Weak Gradient Condition.** We consider the algebraic equation

$$V\psi = k^2\psi_s \tag{65}$$

or

$$V = k^2[(\psi_i^{\pm})^*\psi_s + \mid \psi_s \mid^2]\Psi^{-1} \tag{66}$$

where

$$\Psi^{-1} = \mid \psi \mid^{-2} = \mid \psi_i^{\pm} + \psi_s \mid^{-2} \tag{67}$$

Physically, this result requires that the gradient of the scattered wavefield is significantly smaller than the wavenumber, i.e. for a normal unit vector $\hat{\mathbf{n}}$

$$\mid \hat{\mathbf{n}} \cdot \nabla\psi_s \mid << k \tag{68}$$

which is a 'weak gradient' condition.

REMARK 3.1. Equation (66) relies on on the condition:

$$\mid \psi(\mathbf{r}, k) \mid^2 = \mid \psi_i^{\pm}(\mathbf{r}, k) + \psi_s(\mathbf{r}, k) \mid^2 > 0 \quad \forall \mathbf{r} \in R^3 \tag{69}$$

This condition is satisfied if ψ is a phase only function, i.e.

$$\psi(\mathbf{r}, k) = \exp[i\theta_\psi(\mathbf{r}, k)] \tag{70}$$

where θ_ψ is the phase function which is taken to be a real only function.

3.2. **Fourier Analysis.** Consider equation (66) for the case when $\psi_i^+ = \exp(ik\hat{\mathbf{n}}_i \cdot \mathbf{r})$ and take the Fourier transform with respect to $\mathbf{r}$ for spatial frequencies $k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)$. Using the convolution theorem, i.e.

$$\psi_s^*(\mathbf{r})\psi_s(\mathbf{r}) \leftrightarrow (2\pi)^3\widetilde{\psi}_s^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \circ \widetilde{\psi}_s[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \tag{71}$$

we then obtain

$$\widetilde{V}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \tag{72}$$
$$= k^2 \left\{ \widetilde{\psi}_s(k\hat{\mathbf{n}}_s) + (2\pi)^3 \widetilde{\psi}_s^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \circ \widetilde{\psi}_s[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \right\} \circ \widetilde{\Psi}^{-1}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)]$$

where

$$\widetilde{V}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = \int_{R^3} V(\mathbf{r}) \exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)\cdot \mathbf{r}] d^3\mathbf{r}, \tag{73}$$

$$\begin{aligned} \widetilde{\psi}_s(k\hat{\mathbf{n}}_s) &= \int_{R^3} \psi_s(\mathbf{r},k) \exp(-ik\hat{\mathbf{n}}_i \cdot \mathbf{r}) \exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)\cdot \mathbf{r}] d^3\mathbf{r} \\ &= \int_{R^3} \psi_s(\mathbf{r},k) \exp(-ik\hat{\mathbf{n}}_s \cdot \mathbf{r}) d^3\mathbf{r}, \end{aligned} \tag{74}$$

$$\widetilde{\psi}_s^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = \int_{R^3} \psi_s^*(\mathbf{r}) \exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)\cdot \mathbf{r}] d^3\mathbf{r} \tag{75}$$

and

$$\widetilde{\Psi}^{-1}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = \int_{R^3} \Psi^{-1}(\mathbf{r},k) \exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)\cdot \mathbf{r}] d^3\mathbf{r} \tag{76}$$

CORROLARY 3.1.1. Under the condition $\|\psi_s\|_2 < \|\psi_i^+\|_2$,

$$\begin{aligned} \Psi^{-1}(\mathbf{r}) &= \mid \psi_i^+(\mathbf{r}) + \psi_s(\mathbf{r}) \mid^{-2} \\ &= 1 - 2\psi_i^+(\mathbf{r})\psi_s^*(\mathbf{r}) - 2\psi_s(\mathbf{r})[\psi_i^+(\mathbf{r})]^* - 2 \mid \psi_s(\mathbf{r}) \mid^2 + ... \end{aligned} \tag{77}$$

Thus, noting that

$$\delta^3[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = \frac{1}{(2\pi)^3} \int_{R^3} \exp[ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)\cdot \mathbf{r}] d^3\mathbf{r} \tag{78}$$

and

$$\delta^3[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = \delta^3[-k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \tag{79}$$

and taking the Fourier transform,

$$\begin{aligned} \widetilde{\Psi}^{-1}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] &= (2\pi)^3 \delta^3[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] - 2\widetilde{\psi}_s^*[k(\hat{\mathbf{n}}_s - 2\hat{\mathbf{n}}_i)] \\ &-2\widetilde{\psi}_s(k\hat{\mathbf{n}}_s) - 2\widetilde{\psi}_s[k(\hat{\mathbf{n}}_s - 2\hat{\mathbf{n}}_i)] \circ \widetilde{\psi}_s^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] + ... \end{aligned} \tag{80}$$

and equation (72) can be written as

$$\widetilde{V}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = \tag{81}$$
$$(2\pi)^3 k^2 \left\{ \widetilde{\psi}_s[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] + (2\pi)^3 \widetilde{\psi}_s^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \circ \widetilde{\psi}_s[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \right\} + ...$$

REMARK 3.1.1. Taking the first term on the RHS of equation (81) and ignoring all other terms, we have

$$\widetilde{V}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = (2\pi)^3 k^2 \widetilde{\psi}_s[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \tag{82}$$

This is the case under the assumption that

$$\|\psi_s\|_2 << \|\psi_i\|_2 \tag{83}$$

which is equivalent to equation (34), if $(2\pi)^3 k^2 \widetilde{\psi}_s$ is taken to be equivalent to scattering amplitude defined by equation (34). This observation leads to the following proposition.

PROPOSITION 3.1.1. Under the condition $\|\psi_s\|_2 < \|\psi_i\|_2$, if the function $(2\pi)^3 k^2 \widetilde{\psi}_s$ given in equation (81) is taken to be the scattering amplitude (i.e. when $r_s \to \infty$), then, equation (81) can be considered to provide an inverse scattering solution for the potential

$$V(\mathbf{r}) = \frac{1}{(2\pi)^3} \int_{R^3} \widetilde{V}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \exp[ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i) \cdot \mathbf{r}] d^3[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \tag{84}$$

In otherwords, we consiter the following:

$$(2\pi)^3 k^2 \widetilde{\psi}_s[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \equiv A[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)], \quad r_s \to \infty$$

and

$$(2\pi)^3 k^2 \widetilde{\psi}_s^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \equiv A^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)], \quad r_s \to \infty$$

The rationale for this 'Proposition by Induction' is as follows: Multiplying by ψ_i^+ and then convolving equation (66) with the free space Green's function,

$$g(r,k) \circ V(\mathbf{r}) \exp(ik\hat{\mathbf{n}}_i \cdot \mathbf{r}) = \tag{85}$$

$$k^2 g(r,k) \circ \exp(ik\hat{\mathbf{n}}_i \cdot \mathbf{r}) \{[\exp(-ik\hat{\mathbf{n}}_i \cdot \mathbf{r})\psi_s(\mathbf{r},k) + \mid \psi_s(\mathbf{r},k) \mid^2\} \Psi^{-1}(\mathbf{r},k)$$

and as $r_s \to \infty$,

$$\frac{\exp(ikr_s)}{4\pi r_s} \int_{R^3} V(\mathbf{r}) \exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i) \cdot \mathbf{r}] d^3\mathbf{r} = k^2 \frac{\exp(ikr_s)}{4\pi r_s} \tag{86}$$

$$\times \int_{R^3} \{[\exp(-ik\hat{\mathbf{n}}_i \cdot \mathbf{r})\psi_s(\mathbf{r},k) + \mid \psi_s(\mathbf{r},k) \mid^2\} \Psi^{-1}(\mathbf{r},k) \exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i) \cdot \mathbf{r}] d^3\mathbf{r}$$

which yields equation (72). By this proposition, from equation (81), we consider the equation for the scattering amplitude to be given

$$\widetilde{V}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = A[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] + k^{-2} A^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \circ A[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] + \ldots \tag{87}$$

3.3. **Solution for $\widetilde{\Psi}^{-1} = (2\pi)^3\delta^3$.** The condition

$$\widetilde{\Psi}^{-1}[k(\mathbf{r}_s - \mathbf{r}_i)] = (2\pi)^3\delta^3[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \tag{88}$$

provides an inverse and forward scattering solution that is radically simplified, equation (87) being reduced to

$$\widetilde{V}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = A[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] + k^{-2}A^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \circ A[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \tag{89}$$

so that, for $n = 1, 2, 3, ...$

$$A^{(n+1)}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = \widetilde{V}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] - k^{-2}(A^*)^{(n)}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \circ A^{(n)}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \tag{90}$$

It is then apparent that higher order effects are compounded in a single term, namely, the term

$$(A^*)^{(n)}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \circ A^{(n)}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)]$$

and the Born approximation in the far-field can now be attributed to the case when

$$(A^*)^{(n)}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \circ A^{(n)}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = 0 \tag{91}$$

which 'translates' to the auto-convolution of the scattering amplitude being zero. The physical interpretation of this result is that multiple scattering processes can be expected to produce replicating patterns. These 'matching features' will then contribute to a non-zero auto-convolution function.

REMARK 3.2.1. The condition $\widetilde{\Psi}^{-1} = (2\pi)^3\delta^3$ provide a 'phase-only' solution, i.e. for a unit amplitude, if we assume that $\psi = \exp(i\theta_\psi)$ where θ_ψ is the characteristic phase function, then $\Psi^{-1} = 1$.

REMARK 3.2.2. In 'real-space' equation (90) translates to

$$a^{(n+1)}(\mathbf{r}) = V(\mathbf{r}) - \frac{1}{k^2} \mid a^{(n)}(\mathbf{r}) \mid^2, \quad a^{(1)}(\mathbf{r}) = V(\mathbf{r}) \tag{92}$$

where

$$a^{(n)}(\mathbf{r}) = \frac{1}{(2\pi)^3} \int\limits_{R^3} A^{(n)}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \exp[ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] d^3[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \tag{93}$$

which has the convergence criterion

$$\|a(\mathbf{r})\|_2 < \frac{1}{2} \tag{94}$$

3.4. **Example Application: Rutherford Scattering.** We compute the scattering cross section associated with a screened Coulomb potential $V(r) = \alpha \exp(-ar)/r$ where α is a constant. In this case

$$a^{(1)}(\mathbf{r}) = V(r), \quad A^{(1)}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = \int\limits_{R^3} V(r) \exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] d^3\mathbf{r}, \tag{95}$$

$$a^{(2)}(\mathbf{r}) = V(r) - \frac{1}{k^2} \mid V(r) \mid^2, \tag{96}$$

$$A^{(2)}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] = \int\limits_{R^3} V(r) \exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] d^3\mathbf{r} \tag{97}$$

$$-\frac{1}{k^2} \int\limits_{R^3} \mid V(r) \mid^2 \exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] d^3\mathbf{r},$$

$$a^{(3)}(\mathbf{r}) = V(r) - \frac{1}{k^2} \left[V(r) - \frac{1}{k^2} \mid V(r) \mid^2 \right]^2 \tag{98}$$

and so on. For illustrative purpose, we now consider the computation of just the first and second order terms $a^{(1)}$ and $a^{(2)}$, respectively.

Computation of $A^{(1)}$. Using spherical polar coordinates (r, ϕ, ψ),

$$A^{(1)}(\theta) = \int\limits_0^{2\pi} d\psi \int\limits_{-1}^{1} d(\cos\phi) \int\limits_0^{\infty} dr \;\; r^2 \exp(-ik \mid \hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i \mid r \cos\phi) V(r) \tag{99}$$

Further

$$\mid \hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i \mid = \sqrt{(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i) \cdot (\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)} = \sqrt{2(1 - \cos\theta)}, \quad \cos\theta = \hat{\mathbf{n}}_s \cdot \hat{\mathbf{n}}_i \tag{100}$$

where θ is the scattering angle (the angle between the incident and scattered fields). Using the half angle formula $1 - \cos\theta = 2\sin^2(\theta/2)$ so that $\mid \hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i \mid = 2\sin(\theta/2)$ and integrating over ψ and $\cos\phi$, the scattering amplitude is

$$A^{(1)}(\theta) = \frac{2\pi}{k \sin(\theta/2)} \int\limits_0^{\infty} \sin[2kr\sin(\theta/2)] V(r) r dr \tag{101}$$

For a screened Coulomb potential $V(r) = \alpha \exp(-ar)/r$, the scattering amplitude becomes

$$A^{(1)}(\theta) = \frac{2\alpha\pi}{k\sin(\theta/2)} \int\limits_0^{\infty} \sin[2kr\sin(\theta/2)] \exp(-ar) dr = \frac{\pi\alpha}{k^2 \sin^2(\theta/2)} \tag{102}$$

where we have used the result

$$\int \exp(-ax)\sin(bx) dx = -\frac{\exp(-ax)[a\sin(bx) + b\cos(bx)]}{a^2 + b^2} \tag{103}$$

and then let $a \to 0$. The scattering cross-section is given by

$$| A^{(1)}(\theta) |^2 = \frac{\pi^2\alpha^2}{k^4 \sin^4(\theta/2)} \tag{104}$$

which is the characteristic 'signature' for Rutherford scattering, i.e. scattering from a Coulomb potential.

Computation of $A^{(2)}$. The second term required to compute $A^{(2)}$ is given by

$$\lim_{a\to 0} \frac{2\pi\alpha^2}{k^3\sin(\theta/2)} \int\limits_0^\infty \frac{\sin[2kr\sin(\theta/2)]}{r} \exp(-2ar)dr \tag{105}$$

$$= \frac{2\pi\alpha^2}{k^3\sin(\theta/2)} \int\limits_0^\infty \frac{\sin(x)}{x} dx = \frac{\pi^2}{k^3\sin(\theta/2)}$$

and the scattering cross section is now given by

$$| A^{(2)}(\theta) |^2 = \frac{\pi^2\alpha^2}{k^4} \left| \frac{1}{\sin^2(\theta/2)} - \frac{\pi\alpha}{k\sin(\theta/2)} \right|^2 \tag{106}$$

4. Klein-Gordon Scattering

The Klein-Gordon (KG) equation is a wave equation whose wave function ψ describes spin-less scalar Bosons (such as the Higgs Boson) and is a consequence of applying the energy E and momentum $\mathbf{p}$ operators $E \to i\hbar\partial_t$ and $\mathbf{p} \to -i\hbar\nabla$, respectively, to the relativistic energy equation

$$E^2 = p^2c_0^2 + m^2c_0^4 \tag{107}$$

to give [8]

$$\left(\nabla^2 - \frac{1}{c_0^2}\frac{\partial^2}{\partial t^2}\right)\Psi(\mathbf{r},t) = \frac{m^2c_0^2}{\hbar^2}\Psi(\mathbf{r},t) \tag{108}$$

Using natural units $\hbar = 1$ and $c_0 = 1$ with $\Psi(\mathbf{r},t) = \psi(\mathbf{r},\omega)\exp(\pm i\omega t)$, we can consider the time-independent KG equation

$$\left(\nabla^2 + \omega^2\right)\psi(\mathbf{r},\omega) = m^2\psi(\mathbf{r},\omega) \tag{109}$$

For a potential $V(\mathbf{r})$, the energy is given by $\omega = E - V$ and thus

$$\left[\nabla^2 + (E-V)^2 - E_0^2\right]\psi(\mathbf{r},\omega) = 0 \tag{110}$$

where $E_0 = m$ is the rest-mass energy. This equation can then be written in the form

$$(\nabla^2 + k^2)\psi(\mathbf{r},\omega) = W(\mathbf{r},E)\psi(\mathbf{r},\omega) \tag{111}$$

where $k = \pm\sqrt{E^2 - E_0^2}$ and

$$W = 2E\left(V - \frac{V^2}{2E}\right) \tag{112}$$

is the 'Effective Potential'.

REMARK 4.1. Solutions to this equation are important in the analysis of pionic systems, for example, where the potential V may be real or complex [9]. In many cases, the term V^2/E is neglected on the grounds that the energy range considered is such that V^2/E is small. The omission of this term reduces equation (111) to the Schrödinger equation with an energy-dependent potential. Thus, for $E_0/E << 1$, neglecting the term $V^2/2E$ and with $\psi = \psi_i^\pm + \psi_s$, equation (111) becomes

$$(\nabla^2 + E^2)\psi_s(\mathbf{r}, \omega) = 2EV(\mathbf{r})[\psi_i^\pm(\mathbf{r}, \omega) + \psi_s(\mathbf{r}, \omega)] \tag{113}$$

with

$$(\nabla^2 + E^2)\psi_i(\mathbf{r}, \omega) = 0 \tag{114}$$

In this case, from Theorem 3.1

$$\begin{aligned} 2EV &= \frac{\psi^*}{\mid \psi \mid^2}\nabla^2\left[\psi_s - \frac{E^2}{4\pi r} \circ \psi_s\right] \\ &= \frac{-E^2}{\psi_i^\pm + \psi_s}\psi_s \circ \nabla^2\left(\frac{1}{4\pi r}\right), \quad E \to \infty \\ &= \frac{E^2}{\psi_i^\pm + \psi_s}\psi_s \circ \delta^3 \\ &= E^2\Psi^{-1}[(\psi_i^\pm)^* + \psi_s^*]\psi_s \end{aligned} \tag{115}$$

so that we can then write

$$V = \frac{E}{2}\Psi^{-1}[(\psi_i^\pm)^* + \psi_s^*]\psi_s \tag{116}$$

to which the same analysis used for the Schrödinger equation given in Section 3.2 can be applied (with $k^2 = E/2$).

REMARK 4.2. If the potential V is complex, then the magnitude of the imaginary part can be substantial [10]. This is because the 'effective potential' $W = 2E[V - V^2/(2E)]$ is such that the magnitude of the imaginary part contributes to the real part in determining the effective potential. With $V = V_r + iV_i$, we have

$$W_r = 2E\left(V_r + \frac{(V_i^2 - V_r^2)}{2E}\right) \tag{117}$$

and

$$W_i = 2E\left(V_i - \frac{2V_rV_i}{2E}\right) \tag{118}$$

Thus, if the magnitude of V_i is substantially greater than that of V_r and E, then V_i^2/E becomes the dominant part of W_r and the inclusion of V^2/E in the effective potential becomes necessary.

5. Helmholtz Scattering

Consider the inhomogeneous wave equation for variable wavespeed $c(\mathbf{r})$ given by

$$\left(\nabla^2 - \frac{1}{c^2(\mathbf{r})}\frac{\partial^2}{\partial t^2}\right)\Psi(\mathbf{r},t) = 0 \tag{119}$$

With

$$\frac{1}{c^2(\mathbf{r})} = \frac{1}{c_0^2}[1+\gamma(\mathbf{r})] \tag{120}$$

where c_0 is a constant wave speed, we can write

$$\left(\nabla^2 - \frac{1}{c_0^2(\mathbf{r})}\frac{\partial^2}{\partial t^2}\right)\Psi(\mathbf{r},t) = -\frac{1}{c_0^2}\gamma(\mathbf{r})\frac{\partial^2}{\partial t^2}\Psi(\mathbf{r},t) \tag{121}$$

Thus, with $\Psi(\mathbf{r},t) = \psi(\mathbf{r},\omega)\exp(\pm i\omega t)$ we obtain the inhomogeneous Helmholtz equation given by

$$(\nabla^2 + k^2)\psi(\mathbf{r},k) = -k^2\gamma(\mathbf{r})\psi(\mathbf{r},k) \tag{122}$$

where $k = \omega/c_0$ and γ is the scattering function. Applications of this equation include electromagnetism where ψ denotes the scalar electric wavefield [11]. However, unlike the scattering potential associated with the Schrödinger and Klein-Gordon equations, the scattering function γ is generally taken to be of compact support, i.e. $\gamma(\mathbf{r})$ exists $\forall\mathbf{r} \in \mathcal{D}$. The Green's function transformation for scattering functions that are of compact support must include the surface integral which is taken over the surface of $\mathcal{D}$ so that the transformation becomes

$$\begin{aligned}\psi(\mathbf{r},k) &= k^2 g(r,k)\circ\gamma(\mathbf{r})\psi(\mathbf{r},k)\\ &+ \oint\limits_{\mathcal{S}}[g(r,k)\nabla\psi(\mathbf{r},k) - \psi(\mathbf{r},k)\nabla g(r,k)]\cdot\hat{\mathbf{n}}d^2\mathbf{r}\end{aligned} \tag{123}$$

where $\hat{\mathbf{n}}$ is the unit vector perpendicular to the orientation of the surface element $d^2\mathbf{r}$ and g is the solution of

$$(\nabla^2 + k^2)g(r,k) = -\delta^3(\mathbf{r}) \tag{124}$$

The 'elimination' of the surface integral is based on the following theorem.

THEOREM 5.1. If $\mathbf{r} \in \mathcal{S}$ where $\mathcal{S}$ is the surface of the scattering function γ which is of compact support $\mathbf{r} \in \mathcal{D}$ then, if and only if,

$$\psi(\mathbf{r}, k) = \psi_i^{\pm}(\mathbf{r}, k) \forall \mathbf{r} \in \mathcal{S} \tag{125}$$

where

$$(\nabla^2 + k^2)\psi_i^{\pm} = 0 \tag{126}$$

then

$$\psi(\mathbf{r}, k) = \psi_i^{\pm}(\mathbf{r}, k) + k^2 g(r, k) \circ \gamma(\mathbf{r})\psi(\mathbf{r}, k) \tag{127}$$

Proof. Applying the boundary condition $\psi(\mathbf{r}, k) = \psi_i^{\pm}(\mathbf{r}, k) \forall \mathbf{r} \in \mathcal{S}$, the surface integral becomes

$$\oint_{\mathcal{S}} [g(r, k)\nabla\psi_i^{\pm}(\mathbf{r}, k) - \psi_i^{\pm}(\mathbf{r}, k)\nabla g(r, k)] \cdot \hat{\mathbf{n}} d^2\mathbf{r} \tag{128}$$

$$= \int_{\mathcal{D}} [g(r, k)\nabla^2\psi_i^{\pm}(\mathbf{r}, k) - \psi_i^{\pm}(\mathbf{r}, k)\nabla^2 g(r, k)] d^3\mathbf{r}$$

using Green's Theorem. But since

$$\nabla^2\psi_i^{\pm} = -k^2\psi_i^{\pm} \text{ and } \nabla^2 g(r, k) = -\delta^3(r) - k^2 g(r, k) \tag{129}$$

then

$$\int_{\mathcal{D}} [g(r, k)\nabla^2\psi_i^{\pm}(\mathbf{r}, k) - \psi_i^{\pm}\nabla^2 g(r, k)] d^3\mathbf{r} = \int_{\mathcal{D}} \delta^3(\mathbf{r})\psi_i^{\pm}(\mathbf{r}, k) d^3\mathbf{r} = \psi_i^{\pm}(\mathbf{r}, k) \tag{130}$$

REMARK 5.1 From equation (122), by Theorem 3.1

$$\begin{aligned}
-k^2\gamma &= \frac{\psi^*}{|\psi|^2}\nabla^2\left[\psi_s - \frac{k^2}{4\pi r} \circ \psi_s\right] \\
&= \frac{-k^2}{\psi_i^{\pm} + \psi_s}\psi_s \circ \nabla^2\left(\frac{1}{4\pi r}\right), \quad k \to \infty \\
&= \frac{k^2}{\psi_i^{\pm} + \psi_s}\psi_s \circ \delta^3 \\
&= k^2\Psi^{-1}[(\psi_i^{\pm})^* + \psi_s^*]\psi_s
\end{aligned} \tag{131}$$

and hence

$$\gamma(\mathbf{r}) = -\Psi^{-1}[(\psi_i^{\pm})^* + \psi_s^*]\psi_s \tag{132}$$

6. Conclusion

Formal methods of solution to the forward and inverse Schrödinger scattering problems are based on iterative solutions. The Jost-Kohn method, which is compounded in Lemma 2.3, is based on an iterative inverse scattering solution to an iterative forward scattering solution. This is because the forward scattering problem is solved first which a common theme associated with inverse scattering problems in general.

In this paper, we have developed a 'direct approach' to solving the inverse Schrödinger scattering problem based on Theorem 3.1 and Proposition 3.1.1. The weak gradient condition used to obtain equation (66) is compatible with applications in high energy ion-beam analysis, for example. From an analytical point of view, this condition requires that the scattered field is a smooth function [12]. However, if we relax this condition, then the potential can be written as (for ψ_i^+)

$$V = \Psi^{-1}[(\psi_i^+)^* + \psi_s^*](\nabla^2 + k^2)\psi_s \tag{133}$$

Taking the Fourier transform of this equation for spatial frequencies $k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)$, with Proposition 3.1.1, we obtain

$$\begin{aligned}
\widetilde{V}[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] &= (2\pi)^3 k^2 \{ - \mid \hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i \mid^2 \widetilde{\psi}_s^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \circ \widetilde{\psi}_s[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \\
&+ (2\pi)^3 \widetilde{\psi}_s^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \circ \widetilde{\psi}_s[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)]\} \\
&= -\frac{\mid \hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i \mid^2}{(2\pi)^3 k^2} A^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \circ A[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \\
&+ \frac{1}{k^2} A^*[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \circ A[k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)]
\end{aligned} \tag{134}$$

under the phase only condition

$$\widetilde{\Psi}^{-1} = (2\pi)^3 \delta^3 [k(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i)] \tag{135}$$

We then obtain an 'inverse scattering solution' for V given by

$$V(\mathbf{r}) = \frac{1}{(2\pi)^3 k^2}[\mid a(\mathbf{r}) \mid^2 + k^{-2} a^*(\mathbf{r}) \nabla^2 a(\mathbf{r})] \tag{136}$$

which has a Green's function transformation for a given by

$$a(\mathbf{r}) = \frac{k^2}{4\pi r} \circ a(\mathbf{r}) - \frac{4\pi^2 k^4}{r} \circ \frac{a(\mathbf{r}) V(\mathbf{r})}{\mid a(\mathbf{r}) \mid^2} \tag{137}$$

The forward scattering solutions then rely on iteration. Further by considering equation (77), it is possible to obtain an inverse solution based on an infinite series that is independent of both the weak gradient and phase only conditions, relying solely on Proposition 3.1.1.

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