2009-09-01

Exact Inverse Schrodinger Scattering

Jonathan Blackledge

Dublin Institute of Technology, jonathan.blackledge59@gmail.com

Follow this and additional works at: http://arrow.dit.ie/engscheleart

Exact Inverse Schrödinger Scattering

Jonathan M Blackledge

SFI Stokes Professor
Dublin Institute of Technology
http://eleceng.dit.ie/blackledge

Abstract

The paper briefly reviews the principles of conditional forward and inverse Schrödinger scattering using Rutherford scattering as an example. An approach is considered which, in principle, provides an exact inverse scattering solution from which the scattered field can be computed.

Key words: Inverse Schrödinger scattering, Rutherford scattering, Exact solutions

1. Introduction

For a non-relativistic incident ion beam (described by a unit plane wave function ψ_i), analysis of the scattered field ψ_s generated by the elastic scattering of the beam with a nuclear potential $V(\mathbf{r})$ is determined by solutions to the three dimensional Schrödinger equation

$$(\nabla^2 + k^2)\psi(\mathbf{r}, k) = V(\mathbf{r})\psi(\mathbf{r}, k) \tag{1}$$

where k is the wavenumber and ψ is a complex wavefunction. Let $\psi = \psi_i^{\pm} + \psi_s$ where $(\nabla^2 + k^2)\psi_i^{\pm} = 0$ with solutions $\psi_i^{\pm} = \exp(\pm ik\hat{\mathbf{n}}_i \cdot \mathbf{r})$, $\hat{\mathbf{n}}_i$ being a unit vector that points in the direction of the incident ion beam.

For $V(\mathbf{r}) \to 0$ as $r \equiv \mid \mathbf{r} \mid \to \infty$, the Green's function transformation to equation (1) yields the Lippmann-Schwinger equation [1]

$$\psi(\mathbf{r}, k) = \psi_i^{\pm}(\mathbf{r}, k) + g(r, k) \otimes_3 V(\mathbf{r})\psi(\mathbf{r}, k), \quad g = -\frac{\exp(ikr)}{4\pi r} \tag{2}$$

where $\otimes_3$ denotes the three-dimensional convolution integral and g is the outgoing free space Green's function which is the solution of $(\nabla^2 + k^2)g(r, k) =$

$\delta^3(\mathbf{r})$. A principal aim of ion beam analysis is to infer the characteristics of V by measuring the scattering cross section $|\psi_s|^2$. We present a solution to this problem that is based on the transformation of equation (1) to [2]

$$V(\mathbf{r}) = \frac{\psi^*(\mathbf{r}, k)}{|\psi(\mathbf{r}, k)|^2} \nabla^2 \left(\psi_s(\mathbf{r}, k) - \frac{k^2}{4\pi r} \otimes_3 \psi_s(\mathbf{r}, k) \right) \qquad (3)$$

2. Formal Inverse Solutions

Equation (2) yields the following convergent iterative solution (the Born series) for ψ_s subject to the condition $\|g(r, k) \otimes_3 V(\mathbf{r})\| < 1$:

$$\psi_s(\mathbf{r}, k) = g(r, k) \otimes_3 V(\mathbf{r})\psi_i^\pm(\mathbf{r}, k) + g(r, k) \otimes_3 V(\mathbf{r})[g(r) \otimes_3 V(\mathbf{r})\psi_i^\pm(\mathbf{r}, k)] + ... \qquad (4)$$

$$\sim g(r, k) \otimes_3 V(\mathbf{r})\psi_i^\pm(\mathbf{r}), \quad \|g(r, k) \otimes_3 V(\mathbf{r})\| << 1 \qquad (5)$$

Each term in equation (4) expresses the effects due to single, double, triple, etc. scattering. An inverse scattering solution is achieved by letting $V = c^1 V_1 + c^2 V_2 + ... c^n V_n$ and equating terms with common (real valued) coefficients $c^1, c^2,...$ This provides an iterative solution for computing $V_j, j = 1, 2, ..., n$. V is then obtained from V_j by setting $c = 1$ [3] [4] - an iterative solution to an iterative solution. Equation (5) describes the scattered field generated by single scattering events (the Born approximation) and the inverse problem is compounded in the deconvolution of equation (5) which is a near-field problem. However, when ψ_s is measured in the far-field, for ψ_i^+, the scattered field is given by

$$\psi_s(\mathbf{r}_s, k) \sim -\frac{\exp(ikr_s)}{4\pi r_s} \widetilde{\psi}_s(k\hat{\mathbf{n}}_s), \quad r_s \to \infty$$

where

$$\widetilde{\psi}_s(k\hat{\mathbf{n}}_s) = \int_{-\infty}^{\infty} \exp[-ik(\hat{\mathbf{n}}_s - \hat{\mathbf{n}}_i) \cdot \mathbf{r}]V(\mathbf{r})d^3\mathbf{r} \qquad (6)$$

and $\hat{\mathbf{n}}_s = \mathbf{r}_s/r_s$ is a unit vector that points in the direction of the scattered field. Note that this result is based on equation (5) which, in turn, is based on the equation $V \sim (\psi_i^+)^{-1}(\nabla^2 + k^2)\psi_s$. Also note that, in the far-field, the forward scattering and inverse scattering problems are reduced to forward Fourier and inverse Fourier transformations respectively, i.e. for $\|g(r, k) \otimes_3 V(\mathbf{r})\| << 1$, far-field ion beam analysis is equivalent to Fourier space analysis.

3. Exact Inverse Solution

Since $\|\psi_s - (k^2/4\pi r) \otimes_3 \psi_s\|_2 \leq \|\psi_s\|_2[1 + k^2\sqrt{r/(4\pi)}]$, in the far field, equation (3) becomes

$$V = \frac{-1}{\psi_i^\pm + \psi_s} k^2 \psi_s \otimes_3 \nabla^2 \left(\frac{1}{4\pi r}\right) = k^2 \Psi^{-1}[(\psi_i^\pm)^* + \psi_s^*]\psi_s, \quad r \to \infty \quad (7)$$

where $\Psi^{-1} = \mid \psi_i^\pm + \psi_s \mid^{-2}$. Fourier analysis of equation (7) provides a far-field solution for the scattered field that is compatible with the result given by equation (6) under the Born approximation, i.e. Fourier-space far-field equivalence. Taking the Fourier transform of equation (7) and using the product theorem, for ψ_i^-, we obtain

$$\widetilde{V}(k\hat{\mathbf{n}}) = k^2[\widetilde{\psi}_s[k(\hat{\mathbf{n}}_i - \hat{\mathbf{n}})] + \widetilde{\psi}_s^*(k\hat{\mathbf{n}}) \otimes_3 \widetilde{\psi}_s(k\hat{\mathbf{n}})] \otimes_3 \widetilde{\Psi}^{-1}(k\hat{\mathbf{n}}) \quad (8)$$

where $\hat{\mathbf{n}} = \mathbf{k}/k$ and $\widetilde{\psi}_s$ is taken to be ψ_s in the far field by analogy with equation (6). Since $\Psi^{-1} = 1 - \psi_i^- \psi_s^* - \psi_s(\psi_i^-)^* - \mid \psi_s \mid^2 +...$,

$$\widetilde{\Psi}^{-1}(k\hat{\mathbf{n}}) = \delta^3(k\hat{\mathbf{n}}) - \widetilde{\psi}_s^*[k(\hat{\mathbf{n}}_i + \hat{\mathbf{n}})] - \widetilde{\psi}_s[k(\hat{\mathbf{n}}_i - \hat{\mathbf{n}})] - \widetilde{\psi}_s(k\hat{\mathbf{n}}) \otimes_3 \widetilde{\psi}_s^*(k\hat{\mathbf{n}}) + ...$$

With $\hat{\mathbf{n}}_i - \hat{\mathbf{n}} = \hat{\mathbf{n}}_s$ equation (8) is can be written in the form

$$\widetilde{\psi}_s(k\hat{\mathbf{n}}_s) \otimes_3 \widetilde{\Psi}^{-1}[k(\hat{\mathbf{n}}_i - \hat{\mathbf{n}}_s)] = \frac{\widetilde{V}[k(\hat{\mathbf{n}}_i - \hat{\mathbf{n}}_s)]}{k^2}$$

$$-\widetilde{\psi}_s^*[k(\hat{\mathbf{n}}_i - \hat{\mathbf{n}}_s)] \otimes_3 \widetilde{\psi}_s[k(\hat{\mathbf{n}}_i - \hat{\mathbf{n}}_s)] \otimes_3 \widetilde{\Psi}^{-1}[k(\hat{\mathbf{n}}_i - \hat{\mathbf{n}}_s)] \quad (9)$$

Note that for back-scattering (when $\hat{\mathbf{n}}_i = -\hat{\mathbf{n}}_s$) equation (8) becomes

$$\widetilde{V}(k\hat{\mathbf{n}}_s) = k^2[\widetilde{\psi}_s(-2k\hat{\mathbf{n}}_s) + \widetilde{\psi}_s^*(k\hat{\mathbf{n}}_s) \otimes_3 \widetilde{\psi}_s(k\hat{\mathbf{n}}_s)] \otimes_3 \widetilde{\Psi}^{-1}(k\hat{\mathbf{n}}_s)$$

4. Rutherford Scattering

For a screened Coulomb potential $V(r) = \exp(-ar)/r, a > 0$ - used to obtain a convergent integral in equation (6) - the intensity of the Born scattered field as a function of the scattering angle θ is given by (ignoring scaling)

$$\mid \psi_s(\theta) \mid^2 = \frac{1}{\sin^4(\theta/2)}, \quad a \to 0 \quad (10)$$

which is a characteristic 'signature' of Rutherford scattering. In order to undertake the experiment, Rutherford required a thin foil to generate single scattering events for which Gold leaf offered the best possible technical solution. A thicker foil would have generated multiple scattering leading to an indeterminacy in the results. In this sense, Rutherford's 1909 experiment was designed to interpret Born scattering in the far-field. The method reported in this paper, involves computing the scattered field from the inverse solution given by equation (8) to which different conditions can be applied. For example, the conditions required to obtain equation (10) from equation (9) are $\widetilde{\Psi}^{-1} \sim \delta^3$ and $\widetilde{\psi}_s^* \otimes_3 \widetilde{\psi}_s \sim 0$.

5. Conclusion

The scattering potential is obtained directly from data on the far-scattered-field based on equation (8). The unconditional scattered field is computed using the iteration

$$\widetilde{\psi}_s^{m+1}(k\hat{\mathbf{n}}_s) = \frac{\widetilde{V}[k(\hat{\mathbf{n}}_i - \hat{\mathbf{n}}_s)]}{k^2} \otimes_3 \widetilde{\Psi}^m[k(\hat{\mathbf{n}}_i - \hat{\mathbf{n}}_s)] - \widetilde{\psi}_s^m[k(\hat{\mathbf{n}}_i - \hat{\mathbf{n}}_s)] \otimes_3 (\widetilde{\psi}_s^m)^*[k(\hat{\mathbf{n}}_i - \hat{\mathbf{n}}_s)]$$

where

$$\widetilde{\psi}_s^0(k\hat{\mathbf{n}}_s) = \frac{\widetilde{V}[k(\hat{\mathbf{n}}_i - \hat{\mathbf{n}}_s)]}{k^2}$$

The back-scattered intensity is obtained by computing $\mid \widetilde{\psi}_s^m(k\hat{\mathbf{n}}_s) \mid^2$, $\hat{\mathbf{n}}_s \sim -\hat{\mathbf{n}}_i$ for large m.

References

[1] R. G. Newton, *Inverse Schrodinger Scattering in Three Dimensions*, Springer-Verlag, 1990.

[2] J. M. Blackledge, T. Hämäläinen and J. Joutsensalo, *Inverse Scattering Solutions for Side-Band Signals*, Irish Signals and Systems Conference, June 10-11th, University College Dublin, 2009.

[3] R. Jost and W. Kohn, *Construction of a Potential from a Phase Shift*, Phys. Rev. **37**, 977-992, 1952.

[4] R. T. Prosser, *Formal Solutions of Inverse Scattering Problems*, J. Math. Phys. **17**, 1175-1779, 1976.