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Construction of the Potential of the 3D Schrödinger Equation from the Scattering Operator by Using a Fredholm Integral Equation

Tuncay Aktosun

Department of Mathematical Sciences, University of Texas at Dallas, Richardson, Texas 75083

Cornelis van der Mee

Department of Mathematical Sciences, University of Delaware, Newark, Delaware 19716

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We consider the 3D Schrödinger equation with a potential having no spherical symmetry and show that such a potential can be constructed from the scattering operator by using the solution of a Fredholm integral equation. The Fredholm integral operator presented is compact and self-adjoint; its eigenvalues are symmetric about 0 and lie in $[-1,1]$.

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Consider the Schrödinger equation in three dimensions

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

where k^2 is energy, $\mathbf{x}\in R^3$ is the space coordinate, and $\boldsymbol{\theta}\in S^2$ is a unit vector in R^3. We assume that the potential $V(\mathbf{x})$ is real and decreases to zero sufficiently fast as $|\mathbf{x}|\to\infty$. However, we do not assume any spherical symmetry on the potential. As $|\mathbf{x}|\to\infty$, the wave function $\psi(k,\mathbf{x},\boldsymbol{\theta})$ satisfies

$$\psi(k,\mathbf{x},\boldsymbol{\theta})=e^{ik\boldsymbol{\theta}\cdot\mathbf{x}}+\frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|}A\left(k,\frac{\mathbf{x}}{|\mathbf{x}|},\boldsymbol{\theta}\right)+o\left(\frac{1}{|\mathbf{x}|}\right), \tag{2}$$

where A is the scattering amplitude, which is related to the scattering operator S by

$$S(k,\boldsymbol{\theta},\boldsymbol{\theta}')=\delta(\boldsymbol{\theta}-\boldsymbol{\theta}')-\frac{k}{2\pi i}A(k,\boldsymbol{\theta},\boldsymbol{\theta}'), \tag{3}$$

where δ is the 2D Dirac delta distribution. In operator notation we can write (3) as $S(k)=\mathbf{I}-(k/2\pi i)A(k)$, where the operators act on vectors in $L^2(S^2)$, the Hilbert space of square integrable functions on the unit sphere S^2 in R^3.

The inverse scattering problem is to recover $V(\mathbf{x})$ for all $\mathbf{x}$ when the scattering operator $S(k)$ is known for all k. Since the main source of information about molecular, atomic, and subatomic particles consists of collision experiments, solving the inverse scattering problem is equivalent to determining the forces between particles using the scattering data.

If one assumes that the potential has spherical symmetry, the inverse scattering problem is simplified tremendously, and the potential can be recovered from the so-called phase shifts of the scattering operator. The recovery methods developed in the radial case include the Gel'fand-Levitan[1,2] and Marchenko[2-4] methods. However, in the absence of spherical symmetry, the methods[5-8] that exist to solve the inverse scattering problem are not yet fully developed and there still remain many unanswered questions. For a comprehensive review of the methods and related open problems in 3D inverse scattering theory prior to 1989, the reader is referred to Newton's forthcoming book.[9]

The main idea behind two of the 3D inverse scattering methods, namely the Newton-Marchenko[6] and generalized Gel'fand-Levitan[6] methods, is to formulate the inverse scattering problem as a Riemann-Hilbert boundary-value problem, to transform this Riemann-Hilbert problem into a nonhomogeneous linear integral equation whose kernel is related to the Fourier transform of the scattering data, and to obtain the potential from the resulting integral equation. In this paper we present a

solution of the 3D inverse scattering problem by utilizing a method developed by Muskhelishvili and Vekua[10] to solve a system of Riemann-Hilbert problems with several unknown functions. In the radial case, Newton and Jost[11] used this method to construct potentials from an $n\times n$ scattering matrix. The method we present here generalizes the Muskhelishvili-Vekua method (and hence the Newton-Jost method) to solve an operator Riemann-Hilbert problem for the 3D Schrödinger equation. In the Muskhelishvili-Vekua method the key integral equation has a kernel which is an $(n\times n)$-matrix-valued function whereas in our case we deal with an integral equation whose kernel is an operator-valued function. The Newton-Jost method is restricted to the radial inverse scattering problem for a system of ordinary differential equations with an $n\times n$ scattering matrix; however, in our method we deal with the inverse scattering problem for a partial differential equation with the scattering operator.

The integral operator of our key Fredholm integral equation shares the nice properties of the Newton-Marchenko integral operator[6] such as self-adjointness, compactness, and having an eigenvalue spectrum in $[-1,1]$. Furthermore, our integral operator has a symmetric spectrum about 0, which is not the case for the Newton-Marchenko integral operator. Contrary to the Newton-Marchenko method, we do not use any Fourier transform; the scattering operator is directly used in the kernel of our integral equation whereas one needs to compute the Fourier transform of the scattering operator in order to obtain the kernel of the Newton-Marchenko integral equation.

The results presented in this paper are obtained for potentials that satisfy the following four sufficient conditions. The first two conditions are standard, the third condition is much weaker than usually assumed, and the fourth condition is rather mild.

Definition.—A real potential $V(\mathbf{x})$ is said to belong to the *Newton class* if the following conditions are met: (1)

$$\int d^3x\,|V(\mathbf{x})|\left(\frac{1+|\mathbf{x}|+|\mathbf{y}|}{|\mathbf{x}-\mathbf{y}|}\right)^2\le C<\infty,$$

where the bound C is independent of $\mathbf{y}\in R^3$. (2) $k=0$ is not an exceptional point. (This condition is satisfied if the potential does not have a bound state or half-bound state at zero energy.) (3) There exist constants $c>0$ and $s>\frac{1}{2}$ such that $|V(\mathbf{x})|\le c(1+|\mathbf{x}|^2)^{-s}$ for all $\mathbf{x}\in R^3$. (4) There exists a constant $\beta>0$ such that $\int d^3x\,|\mathbf{x}|^\beta|V(\mathbf{x})|<\infty$.

In the Schrödinger equation k appears as k^2 and hence $\psi(-k,\mathbf{x},\boldsymbol{\theta})$ is a solution whenever $\psi(k,\mathbf{x},\boldsymbol{\theta})$ is. These two solutions are related to each other as[6]

$$\psi(k,\mathbf{x},\boldsymbol{\theta})=\int_{S^2}d\boldsymbol{\theta}'\,S(k,-\boldsymbol{\theta},\boldsymbol{\theta}')\psi(-k,\mathbf{x},\boldsymbol{\theta}'). \tag{4}$$

Letting

$$X_\pm(k,\mathbf{x},\boldsymbol{\theta})=e^{\pm ik\boldsymbol{\theta}\cdot\mathbf{x}}\psi(\pm k,\mathbf{x},\pm\boldsymbol{\theta})-1 \tag{5}$$

and

$$G(k,\mathbf{x},\boldsymbol{\theta},\boldsymbol{\theta}')=e^{-ik\boldsymbol{\theta}\cdot\mathbf{x}}S(k,-\boldsymbol{\theta},-\boldsymbol{\theta}')e^{ik\boldsymbol{\theta}'\cdot\mathbf{x}}, \tag{6}$$

we can write (4) in the operator form as

$$X_+(k,\mathbf{x})=G(k,\mathbf{x})X_-(k,\mathbf{x})+[G(k,\mathbf{x})-\mathbf{I}]\hat{1},\quad k\in R, \tag{7}$$

where $\hat{1}$ is the function defined as $\hat{1}(\boldsymbol{\theta})=1$ for all $\boldsymbol{\theta}\in S^2$.

If there are no bound states and if the potential satisfies the first condition in the definition of the Newton class, then for each $\mathbf{x}$, $X_+(k)$ has an analytic extension in k to C^+, the complex upper half plane, and $X_+(k)\to 0$ as $k\to\infty$ there. Similarly, $X_-(k)$ has an analytic extension in k to C^-, the lower half plane, and vanishes as $k\to\infty$ there. Then, from the Cauchy integral formula we have

$$X_+(k,\mathbf{x})=\frac{1}{\pi i}\mathrm{P}_C\int_{-\infty}^{\infty}dt\,\frac{X_+(t,\mathbf{x})}{t-k} \tag{8}$$

and

$$X_-(k,\mathbf{x})=\frac{-1}{\pi i}\mathrm{P}_C\int_{-\infty}^{\infty}dt\,\frac{X_-(t,\mathbf{x})}{t-k}, \tag{9}$$

where P_C stands for the Cauchy principal value. Operating on (9) by $G(k,\mathbf{x})$ given in (6), adding the result to (8), and rearranging the terms, we obtain the integral equation

$$X_+(k,\mathbf{x})-\mathrm{P}_C\int_{-\infty}^{\infty}dt\,K(k,t;\mathbf{x})X_+(t,\mathbf{x})=H(k,\mathbf{x}), \tag{10}$$

where

$$K(k,t;\mathbf{x})=\frac{1}{2\pi i}\frac{\mathbf{I}-G(k,\mathbf{x})G(t,\mathbf{x})^{-1}}{t-k} \tag{11}$$

and

$$H(k,\mathbf{x})=\left[G(k,\mathbf{x})-\mathbf{I}+\int_{-\infty}^{\infty}K(k,t;\mathbf{x})dt\right]\hat{1}.$$

For potentials in the Newton class, $G(k,\mathbf{x})$ is Hölder continuous in k with a positive exponent[12] and thus the integral in (10) is not singular; i.e., $K(k,t;\mathbf{x})$ does not blow up as $t\to k$. Thus, (10) is a regular Fredholm integral equation and P_C can be dropped in front of the integral there.

The Möbius transformation $k\to\xi=(k-i)/(k+i)$ maps the extended real axis onto the unit circle T on the complex ξ plane. Under this transformation C^+ is mapped onto the interior of the unit circle and C^- is mapped onto the exterior of the unit circle. Using $\xi=(k-i)/(k+i)$ and $\eta=(t-i)/(t+i)$, the Fredholm integral equation (10) is transformed onto the unit circle

and becomes

$$Y(\xi,\mathbf{x})-\oint_T d\eta\,\tilde{K}(\xi,\eta;\mathbf{x})Y(\eta,\mathbf{x})=L(\xi,\mathbf{x})\,, \tag{12}$$

where $L(\xi,\mathbf{x})=[(k+i)/2i]H(k,\mathbf{x})$ and $\tilde{K}(\xi,\eta;\mathbf{x})=H(k,t;\mathbf{x})$ and

$$Y(\xi,\mathbf{x})=\frac{k+i}{2i}X_+(k,\mathbf{x})\,. \tag{13}$$

For potentials in the Newton class, we establish the following results:

Theorem 1.—The Fredholm integral operator $\tilde{K}$ in (12) is compact and self-adjoint; its eigenvalues belong to $[-1,1]$ and are symmetrically located around 0.

Theorem 2.—If $X_\pm(k,\mathbf{x})$ is a solution of the Riemann-Hilbert problem (7), then $X_+(k,\mathbf{x})$ is a solution of the Fredholm equation (10) and $Y(\xi,\mathbf{x})$ obtained from (13) is a solution of the Fredholm equation (12). Conversely, if $X_+(k,\mathbf{x})$ is a solution of (10) and if $X_+(k,\mathbf{x})$ has an analytic extension in k to C^+, then it is also a solution of (7).

If ± 1 are not eigenvalues of $\tilde{K}$, the Fredholm equation (12) or equivalently (10) can be solved uniquely by using iteration. A simple sufficient condition that ± 1 are not eigenvalues is given by $\max_{k\in R}\|S(k)-\mathbf{I}\|<1$. Note that, as seen from Theorem 1 above, -1 is an eigenvalue if and only if $+1$ is an eigenvalue.

The solution of the inverse scattering problem can be obtained from the solution $Y(\xi,\mathbf{x})$ of the Fredholm equation (12) as follows. Using (13) one obtains

$$X_+(k,\mathbf{x})=\frac{2i}{k+i}Y\left(\frac{k-i}{k+i},\mathbf{x}\right),$$

and in the case that $X_+(k,\mathbf{x})$ is analytic for $k\in C^+$, one recovers the potential from (1) as

$$V(\mathbf{x})=\frac{[\nabla^2+2ik\boldsymbol{\theta}\cdot\nabla]X_+(k,\mathbf{x},\boldsymbol{\theta})}{1+X_+(k,\mathbf{x},\boldsymbol{\theta})} \tag{14}$$

provided the right-hand side is independent of k and $\boldsymbol{\theta}$. It can be shown[12] that whenever the so-called miracle condition of Newton[6] is satisfied, the right-hand side of (14) is independent of k and $\boldsymbol{\theta}$. The integral equation (12) or equivalently (10) is uniquely solvable if and only if the Riemann-Hilbert problem (7) is uniquely solvable; when this happens, for the class of scattering operators that are associated with a potential in the Newton class, it is guaranteed that the right-hand side of (14) is independent of k and $\boldsymbol{\theta}$. Note also that, in the case that (10) does not have a solution $X_+(k,\mathbf{x})$ which is analytic for $k\in C^+$, one can conclude immediately, even without evaluating the right-hand side of (14), that a potential does not exist. In other words, the analyticity mentioned in Theorem 2 is a prerequisite for the satisfaction of the miracle condition of Newton.

If the potential $V(\mathbf{x})$ has any bound states, each bound state corresponds to a simple pole of $X_+(k,\mathbf{x},\boldsymbol{\theta})$ on the positive imaginary axis in the complex k plane. These poles can be removed from the scattering operator by the reduction method of Newton[6] before our method is applied. All the proofs and the mathematical details of the method outlined in this paper with and without bound states will be published elsewhere.[13]

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[1]I. M. Gel'fand and B. M. Levitan, Amer. Math. Soc. Transl. **1**, 253 (1955).

[2]K. Chadan and P. C. Sabatier, *Inverse Problems in Quantum Scattering Theory* (Springer-Verlag, New York, 1989), 2nd ed.

[3]Z. S. Agranovich and V. A. Marchenko, *The Inverse Problem of Scattering Theory* (Gordon and Breach, New York, 1963).

[4]L. D. Faddeev, J. Math. Phys. **4**, 72 (1963).

[5]L. D. Faddeev, J. Sov. Math. **5**, 334 (1976); R. G. Newton, Inverse Problems **1**, 371 (1985).

[6]R. G. Newton, J. Math. Phys. **21**, 1698 (1980) [addenda **22**, 631 (1981); **23**, 693 (1982)]; **22**, 2191 (1981) [addendum **23**, 693 (1982)]; **23**, 2257 (1982).

[7]A. I. Nachman and M. J. Ablowitz, Stud. Appl. Math. **71**, 243 (1984); R. Beals and R. R. Coifman, Physica (Amsterdam) **18D**, 242 (1986).

[8]R. T. Prosser, J. Math. Phys. **10**, 1819 (1969); **17**, 1775 (1976); **21**, 2648 (1980); **23**, 2127 (1982).

[9]R. G. Newton, "Inverse Schrödinger Scattering in Three Dimensions" (Springer-Verlag, New York, to be published).

[10]N. I. Muskhelishvili and N. P. Vekua, Tr. Tbilis. Mat. Inst. **12**, 1 (1943) (Russian); *Singular Integral Equations* (Noordhoff, Groningen, 1953).

[11]R. G. Newton and R. Jost, Nuovo Cimento **1**, 590 (1955).

[12]T. Aktosun and C. van der Mee, "Solution of the Inverse Scattering Problem for the 3-D Schrödinger Equation by Wierner-Hopf Factorization of the Scattering Operator" (to be published).

[13]T. Aktosun and C. van der Mee, "Solution of the Inverse Scattering Problem for the 3-D Schrödinger Equation Using a Fredholm Integral Equation" (to be published).