Existence of the Jost Operator and Solution of the 3D Inverse Scattering Problem by Wiener-Hopf Factorization

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We establish three results in the 3D Schrödinger equation with a potential having no spherical symmetry: the existence of a Wiener-Hopf factorization of the scattering operator, a method to recover the potential from the scattering data, and the existence of the 3D Jost operator.

Consider the Schrödinger equation in three dimensions

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

where k^2 is energy, $\mathbf{x} \in \mathbf{R}^3$ is the space coordinate, and $\theta \in S^2$ is a unit vector in $\mathbf{R}^3$. The potential $V(\mathbf{x})$ is real and is assumed to decrease to zero fast enough as $|\mathbf{x}| \to \infty$, but it is not assumed to have any spherical symmetry. As $|\mathbf{x}| \to \infty$, the wave function satisfies

$$\psi(k,\theta,\mathbf{x}) = e^{ik\theta\mathbf{x}} + \frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|} A\left[k, \frac{\mathbf{x}}{|\mathbf{x}|}, \theta\right] + O(1) , \quad (2)$$

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

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

and $\delta(\theta - \theta')$ is the 2D Dirac δ distribution. In operator notation we have $S(k) = I - (k/2\pi i)A(k)$, 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 $\mathbf{R}^3$.

The direct scattering problem is to obtain $S(k)$ when the potential $V(\mathbf{x})$ is given. The inverse scattering problem, however, is to recover $V(\mathbf{x})$ from $S(k)$. The main source of information about molecular, atomic, and subatomic particles consists of collision experiments; hence, the solution of the inverse scattering problem is equivalent to the determination of the forces between particles using the scattering data and is of the utmost importance in physics. The methods developed to solve

the 3D inverse scattering problem include the Newton-Marchenko method,[1] the Gel'fand-Levitan method,[1] the $\bar{\partial}$ method,[2] a method that relies only on backward scattering data,[3] and a method that uses the Green's function of Faddeev.[4,5] However, there are still many open problems in 3D inverse scattering theory, and the methods developed are far from complete. A comprehensive and up-to-date review of the methods and related open problems in 3D inverse scattering theory can be found in a forthcoming book on Newton.[6]

The main idea behind the Newton-Marchenko and Gel'fand-Levitan methods[1] 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 scattering data, and to obtain the potential from the resulting integral equation.

In this paper we present a solution method for the 3D inverse scattering problem by establishing a Wiener-Hopf factorization of the scattering operator, and thus by solving the Riemann-Hilbert problem. The usual theory of Wiener-Hopf factorization, however, deals with either scalar functions[7] or square matrix functions.[8] Here we give the Wiener-Hopf factorization of the scattering operator in an infinite-dimensional setting[9] by using some results of Gohberg and Leiterer.[10]

The results presented in this paper are obtained for potentials that satisfy the following four sufficient conditions. The first two conditions below are standard and

the third condition is much weaker than usually assumed.[6] Our fourth condition is rather mild.

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

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

where the bound C is independent of $\mathbf{y} \in \mathbf{R}^3$. (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 $c>0$ and $s>\frac{1}{2}$ such that $|V(\mathbf{x})| \le c(1+|\mathbf{x}|^2)^{-s}$ for all $\mathbf{x} \in \mathbf{R}^3$. (4) There exists $\beta > 0$ such that $\int_{\mathbf{R}^3} d^3x \, |\mathbf{x}|^\beta |V(\mathbf{x})| < \infty$.

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

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

Let

$$X_+(k,\theta,\mathbf{x}) = e^{-ik\theta\mathbf{x}} \psi(k,\theta,\mathbf{x}) - 1 , \quad (5)$$

$$X_-(k,\theta,\mathbf{x}) = e^{-ik\theta\mathbf{x}} \psi(-k,-\theta,\mathbf{x}) - 1 , \quad (6)$$

$$G(k,\theta,\theta',\mathbf{x}) = e^{-ik\theta\mathbf{x}} S(k,-\theta,-\theta') e^{ik\theta'\mathbf{x}} . \quad (7)$$

Then (5) can be written as

$$X_+(k) = G(k) X_-(k) + [G(k) - \mathbf{I}] \hat{1} , \quad (8)$$

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

It is known[1] that in the absence of bound states

$$X_+(k) = [G_+(k) - \mathbf{I}] \hat{1} + G_+(k) \sum_{\rho_j > 0} \frac{\phi_j(k)}{(k+i)^{\rho_j}} \pi_j , \quad (11)$$

$$X_-(k) = [G_-(k)^{-1} - \mathbf{I}] + G_-(k)^{-1} \sum_{\rho_j > 0} \frac{\phi_j(k) + [(k+i)^{\rho_j} - (k-i)^{\rho_j}] P_j \hat{1}}{(k-i)^{\rho_j}} , \quad (12)$$

provided $P_j \hat{1} = 0$ whenever $\rho_j < 0$. Here π_j is a fixed nonzero vector in the range of P_j and $\phi_j(k)$ is an arbitrary polynomial of degree less than ρ_j. Using the Schrödinger equation the potential is then obtained as[11]

$$V(\mathbf{x}) = \frac{(\nabla^2 + 2ik\theta\nabla) X_+(k,\theta,\mathbf{x})}{1 + X_+(k,\theta,\mathbf{x})} , \quad (13)$$

provided the right-hand side is independent of k and θ. It can be shown[11] that the k and θ independence of the

$X_+(k)$ has an analytic extension in k to $\mathbf{C}^+$, the complex upper half-plane, and $X_+(k) \to 0$ as $k \to \infty$ in $\mathbf{C}^+$. Similarly, $X_-(k)$ has an analytic extension in k to $\mathbf{C}^-$, the lower half-plane, and $X_-(k) \to 0$ as $k \to \infty$ in $\mathbf{C}^-$. The Riemann-Hilbert problem amounts to determining $X_+(k)$ and $X_-(k)$ from $G(k)$. Once $X_+(k)$ and $X_-(k)$ are found, one obtains a solution of the Schrödinger equation and hence, in principle, the potential.

We establish the following result.

Theorem 1.— If the potential $V(\mathbf{x})$ belongs to the Newton class, the operator function $G(k)$ defined in (7) has a Wiener-Hopf factorization, i.e.,

$$G(k) = G_+(k) D(k) G_-(k) , \quad (9)$$

where $G_+(k)$ is an operator function having an analytic extension to $\mathbf{C}^+$, $G_+(k)^{-1}$ exists there as a bounded operator, and $G_+(k) \to \mathbf{I}$ on $\mathbf{C}^+$ in operator norm. Similarly, $G_-(k)$ is an operator function with an analytic extension to $\mathbf{C}^-$, $G_-(k)^{-1}$ exists there as a bounded operator, and $G_-(k) \to \mathbf{I}$ on $\mathbf{C}^-$ in operator norm. The diagonal operator $D(k)$ is given by

$$D(k) = P_0 + \sum_{j=1}^m \left[\frac{k-i}{k+i} \right]^{\rho_j} P_j , \quad (10)$$

where $P_1, \ldots, P_m$ are finitely many, mutually disjoint rank-one projections and $P_0 = \mathbf{I} - \sum_{j=1}^m P_j$. The numbers $\rho_1, \ldots, \rho_m$ are nonzero integers called the partial indices of $G(k)$.

Using the Wiener-Hopf factorization given above, the solution of (8) is given by[11]

right-hand side of (13) is equivalent to the so-called miracle condition of Newton.[1]

The vector Riemann-Hilbert problem (8) is associated with the operator Riemann-Hilbert problem

$$\mathbf{X}_+(k) = G(k) \mathbf{X}_-(k) + G(k) - \mathbf{I} . \quad (14)$$

Using the Wiener-Hopf factorization of $G(k)$ given in (9), the solution of (14) is obtain as[11]

$$\mathbf{X}_+(k) = [G_+(k) - \mathbf{I}] + G_+(k) \sum_{\rho_j > 0} \frac{\phi_j(k)}{(k+i)^{\rho_j}} P_j , \quad (15)$$

$$\mathbf{X}_-(k) = [G_-(k)^{-1} - \mathbf{I}] + G_-(k)^{-1} \sum_{\rho_j > 0} \frac{\phi_j(k) + [(k+i)^{\rho_j} - (k-i)^{\rho_j}]}{(k-i)^{\rho_j}} P_j , \quad (16)$$

provided there are no negative partial indices. If there are negative partial indices, the solution to (14) does not exist. Again $\phi_j(k)$ is an arbitrary polynomial of degree less than ρ_j.

When $\mathbf{x} = 0$, the operator $[\mathbf{I} + \mathbf{X}_+(k)]^{-1}$ becomes the Jost operator used in the 3D Gel'fand-Levitan inversion

method.[1] The existence of the Jost operator has been an open question,[1] which has now been resolved for potentials in the Newton class.

Thus we have the following result.

Theorem 2.—If the potential $V(\mathbf{x})$ belongs to the Newton class, the Jost operator exists if and only if there are no negative partial indices. In that case the Jost operator is given by[11]

$$J(k) = \left[\mathbf{I} - \sum_{\rho_j > 0} \frac{\omega_j(k) - (k+i)^{\rho_j}}{\omega_j(k)} P_j \right] QS_+(k)^{-1}Q,$$

(17)

where, for all $\rho_j > 0$, $\omega_j(k)$ is an arbitrary polynomial of degree equal to ρ_j with leading coefficient 1 and without zeros in $\mathbf{C}^+ \cup \mathbf{R}$. $S_+(k)$ is one of the factors in the Wiener-Hopf factorization $S(k) = S_+(k)D(k)S_-(k)$ of the scattering operator $S(k)$. In the absence of partial indices, the Jost operator is uniquely given by $QS_+(k)^{-1}Q$.

If the potential $V(\mathbf{x})$ has any bound states, each bound state corresponds to a simple pole $X_+(k,\theta,\mathbf{x})$ given in (5) on the positive imaginary axis in the complex k plane.[1] It is possible to use the reduction method of Newton[1] to remove these bound state poles from the scattering operator. Then the Wiener-Hopf factorization method described above can be used to solve the Riemann-Hilbert problems (8) and (14), to solve the inverse scattering problem, and to find the Jost operator. All the proofs and the mathematical details of the method outlined in this paper with and without bound states will be published elsewhere.[11]

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