JOURNAL OF COMPUTATIONAL PHYSICS 97, 516–534 (1991)

Quantum Inverse Scattering Problem as a Cauchy Problem

D. I. ABRAMOV

Department of Theoretical Physics,
Leningrad State University, 198904 Leningrad, USSR

Received December 13, 1988; revised May 22, 1990

An approach to the inverse problem of quantum scattering at fixed angular momentum l using new nonlinear equations is proposed. In this approach, energy levels, normalization constants, and the Jost function of the problem on the interval with a variable left bounary $[r, \infty)$ are considered. These functions as functions of r numbered by energy E as an index (discrete or continuous) satisfy the infinite system of ordinary first-order differential equations. The scattering data serve as initial conditions for this system, and the inverse scattering problem is reduced to the Cauchy problem. As the functions considered in our treatment are slowly varying functions of r, the equations presented here are convenient for practical calculations. Some numerical examples show that the problem of reconstruction of the potential can be solved with high accuracy even with the simplest algorithms. © 1991 Academic Press, Inc.

1. INTRODUCTION

Transformation of the linear Schrödinger equation into the non-linear Milne equation for the wave function amplitude is widely used in the direct problem of quantum mechanics, i.e., in the calculation of energy levels and scattering phaseshifts in a given field [1–5]. The advantages of this approach are connected with the fact that the wave function amplitude is slowly varying, contrary to the wave function itself. The same advantages are typical of different versions of the phase-function method based on numerical integration of the non-linear phase equation [6, 7].

A similar approach is proposed in the present paper to the inverse problem of quantum scattering at fixed angular momentum l. This problem consists in reconstruction of the central potential $U(r)$ when scattering data—phaseshift $\eta(E)$ $(0 \leqslant E < \infty)$, energy levels E_n, and normalization constants C_n—are known for given l. The approach presented differs principally from the traditional Gel'fand–Levitan method [8, 9] and generalizes the results of [10]. It is based on the new exact system of equations for solution of the reduced inverse problem. This system consists of the non-linear ordinary first-order differential equations for the slowly varying functions of variable r—$|F(E, r)|$, $E_n(r)$, and $C_n(r)$ $(0 \leqslant E < \infty$, $n = 1, 2, ..., N(r))$. Here $|F(E, r)|$, $E_n(r)$, and $C_n(r)$ are the modulus of the Jost func-

0021-9991/91 $3.00
Copyright © 1991 by Academic Press, Inc.
All rights of reproduction in any form reserved.

tion, the nth energy level, and the nth normalization constant, corresponding to quantization in the field $U(x)$ on the interval $r \leqslant x < \infty$. Energy E plays, in fact, the role of the index which numbers the unknown functions: the usual summation corresponds to the discrete spectrum and integration over E to the continuous one. When $r \to 0$ then $|F(E, r)| \to |F(E)|$, $E_n(r) \to E_n$, $C_n(r) \to C_n$, where $|F(E)|$, E_n, C_n are the usual set of scattering data. So we see that they serve as initial conditions for our system and thus the inverse problem is reduced to the Cauchy problem.

As the functions $|F(E, r)|$, $E_n(r)$, $C_n(r)$ are uniquely connected with the spectral density $\rho(E, r)$ of the Schrödinger operator on the interval $[r, \infty)$, our system can be considered as a non-linear equation for $\rho(E, r)$. The inverse scattering problem is equivalent to the initial-value problem for this equation, as $\rho(E, 0)$ is expressed in terms of scattering data.

In the simplest case—when bound states are absent—our system converts to the integro-differential equation for the amplitude of the Jost solution which was obtained by the author earlier for the case $l = 0$ [10].

The mathematical problems connected with the proof of the unique existence of the solution for the non-linear system presented require a special investigation and are not discussed here.

To detemine the efficiency of our approach the test numerical calculations have been performed for different cases. They show that the potential may be reconstructed by our method with high accuracy even if the simplest calculation algorithms are used.

2. Principal Notations

Let a central potential $U(r)$ decrease faster than r^{-2} as $r \to \infty$. In the system where $\hbar = 1$, $2m = 1$ (m being the mass of the particle), the radial Schrödinger equation reads

$$f''(r) + [E - l(l+1)\, r^{-2} - U(r)]\, f(r) = 0. \tag{1}$$

The Jost solution of (1) is fixed by the condition

$$f_l(E, r) \underset{r \to \infty}{=} \exp(ikr), \tag{2}$$

where $k = E^{1/2}$. The notation $f_l^0(E, r)$ is used for the Jost solution corresponding to $U(r) \equiv 0$:

$$f_l^0(E, r) = \exp[i\pi(l+1)/2](\pi kr/2)^{1/2} H^{(1)}_{l+1/2}(kr). \tag{3}$$

Here $H_\nu^{(1)}(z)$ is the Hankel function [11].

As the angular momentum l is fixed we shall omit index l for brevity everywhere except in Eqs. (25)–(27) and (33)–(36):

$$f_l(E, r) \equiv f(E, r), \qquad f_l^0(E, r) \equiv f^0(E, r).$$

The Jost function $F(E) \equiv F_l(E)$ is defined by the relation [8]

$$F(E) = |F(E)| \exp[-i\eta(E)] = \lim_{r \to 0} f(E, r)/f^0(E, r), \tag{4}$$

$\eta(E) \equiv \eta_l(E)$ being the scattering phase shift.

Let $\varphi(E, r) \equiv \varphi_l(E, r)$ be the solution of (1) which satisfies the boundary condition at $r = 0$:

$$\varphi(E, r) \underset{r \to 0}{=} r^{l+1}/(2l+1)!!. \tag{5}$$

In the continuous spectrum ($E > 0$) we have

$$\begin{aligned} &\varphi(E, r) = \frac{1}{2ik^{l+1}} \left[f(E, r)\, F^*(E) \exp\left(-\frac{\pi i l}{2}\right) - f^*(E, r)\, F(E) \exp\left(\frac{i\pi l}{2}\right) \right] \\ &\varphi(E, r) \underset{r \to \infty}{=} |F(E)|\, k^{-l-1} \sin(kr + \eta - \pi l/2) \end{aligned} \tag{6}$$

(f^* denotes the complex conjugation of f). In the discrete spectrum the bound state with energy $E_n \equiv E_{nl} < 0$ is described by the eigenfunction $\varphi_n(r) \equiv \varphi(E_n, r)$. The corresponding normalization constant is given by

$$C_n = \int_0^\infty \varphi_n^2(r)\, dr, \qquad n = 1, 2, ..., N. \tag{7}$$

The inverse scattering problem with l fixed consists in the reconstruction of the potential $U(r)$ when $|F(E)|$, E_n, and C_n are known for this l, for all $E \in [0, \infty)$ and $n = 1, 2, ..., N$. Because of the known dispersion relation between modulus and phase of the Jost function [8],

$$\ln |F(E)| = \sum_{n=1}^{N} \ln(1 - E_n/E) - \frac{1}{\pi} \int_0^\infty \frac{\eta(\tilde{E})\, d\tilde{E}}{\tilde{E} - E}, \qquad E \in [0, \infty) \tag{8}$$

($\int_0^\infty$ is the principal value of the integral), one may consider the function $|F(E)|$, given instead of $\eta(E)$. In other words, the spectral density $\rho(E)$ defined by

$$\rho(E) = \begin{cases} E^{l+1/2} \pi^{-1} |F(E)|^{-2}, & E > 0 \\ \sum_{j=1}^{N} C_j^{-1}\, \delta(E - E_j), & E < 0 \end{cases}$$

$$\int_{-\infty}^{\infty} \varphi(E, r)\, \varphi(E, r')\, \rho(E)\, dE = \delta(r - r'),$$

where $\delta(x)$ is the delta function, serves as the input data for the problem under consideration.

Let $E_n(r)$ be the root of $f(E, r)$ as a function of E:

$$f(E_n(r), r) \equiv 0, \qquad E_n(r) < 0, \qquad n = 1, 2, ..., N(r).$$

It is evident that $E_n(r)$ is the energy of nth bound state in the field $U(x)$ when the interval of quantization is $x \in [r, \infty)$, i.e., when the motion is restricted at $x = r$ by an infinite wall. At $r = 0$ these levels coincide with the initial levels $E_n(0) = E_n$. They increase monotonically with r and merge with continuum at some $r = r_n$:

$$E_n(r_n) = 0.$$

The approach presented in this paper is founded on the system of equations for $|f(E, r)|$ and $E_n(r)$. It is convenient, however, to transform this system into the system for functions $|F(E, r)|$, $E_n(r)$, and $C_n(r)$, where

$$\begin{aligned} F(E, r) &= f(E, r)/f^0(E, r) \\ C_n(r) &= [E_n'(r)]^{-1} |E_n(r)|^{-l} [f^0(E_n(r), r)]^{-2}. \end{aligned} \tag{9}$$

The functions $F(E, r)$, $E_n(r)$, $C_n(r)$ are the Jost function, the energy of the nth bound state, and the nth normalization constant, respectively, for the scattering problem on the interval $[r, \infty)$. Instead of (5) we now have the solution of the Schrödinger equation $\varphi(r, E; x)$ (x is an independent variable, r is a parameter indicating the left boundary of the interval) which satisfies the initial conditions

$$\begin{aligned} \varphi(r, E; x)|_{x=r} &= 0 \\ \frac{\partial}{\partial x} \varphi(r, E; x)|_{x=r} &= |E|^{l/2} |f^0(E, r)|^{-1}. \end{aligned} \tag{10}$$

In the discrete spectrum the nth eigenfunction is $\varphi_n(r, x) = \varphi(r, E_n(r); x)$, while $C_n(r)$ (9) is the normalization constant for $\varphi_n(r, x)$. Indeed, $\varphi_n(r, x)$ is given by

$$\varphi_n(r, x) = |E|^{-l/2} |f^0(E, r)|^{-1} [f'(E, r)]^{-1} f(E, x)|_{E = E_n(r)}.$$

Taking into account the relations

$$\begin{aligned} \int_r^\infty f^2(E, x)\, dx &= f(E, r)\, \dot{f}'(E, r) - f'(E, r)\, \dot{f}(E, r) \\ E_n'(r) &= -f'(E, r)/\dot{f}(E, r)|_{E = E_n(r)}, \end{aligned} \tag{11}$$

where

$$f'(E, r) = \partial f(E, r)/\partial r, \qquad \dot{f}(E, r) = \partial f(E, r)|\partial E,$$

we have

$$\int_r^\infty \varphi_n^2(r, x)\, dx = |E_n(r)|^{-l} |f^0(E_n(r), r)|^{-2} [E_n'(r)]^{-1} = C_n(r). \tag{12}$$

It is evident that functions $|F(E, r)|$, $E_n(r)$, $C_n(r)$, which play the central role in our approach, are connected with the spectral density $\rho(E, r)$ of the problem (1), (10) on the interval $[r, \infty)$:

$$\rho(E, r) = \begin{cases} E^{l+1/2}\pi^{-1}\,|F(E, r)|^{-2}, & E>0 \\ \sum_{j=1}^{N(r)} C_j^{-1}(r)\,\delta(E-E_j(r)), & E<0 \end{cases}$$
$$\int_{-\infty}^{\infty} \varphi(r, E; x)\,\varphi(r, E; x')\,\rho(E, r)\,dE = \delta(x-x'). \tag{13}$$

In the limit $r \to 0$ the functions $F(E, r)$, $E_n(r)$, $C_n(r)$ are equal to $F(E)$, E_n, C_n (7), respectively:

$$F(E, 0) = F(E), \qquad E_n(0) = E_n, \qquad C_n(0) = C_n. \tag{14}$$

For $F(E, r)$ and $E_n(r)$, it is obvious. For $C_n(r)$, it follows from the equality

$$\lim_{r \to 0} \varphi(r, E; x) = \varphi(E, x),$$

where $-\infty < E < \infty$ and $\varphi(E, r)$ is fixed by (5). To prove the last equality it is enough to check only that the following limiting transition for Wronskians is true:

$$[\varphi(r, E; x), f(E, x)] = -f(E, r)\,|E|^{-1/2}\,|f^0(E, r)|^{-1} \underset{r \to 0}{=} [\varphi(E, x), f(E, x)].$$

3. Reduction of the Inverse Problem to the Initial-Value Problem

The principal moment of our derivation is the dispersion relation for function $F(E, r)$ which is similar to (8) and is obtained in the same way. It is known [8] that $f(E, r)$ is an analytical function of E in the complex plane with the cut along positive real axis. All its roots are situated on the negative real axis. At large E this function has the following asymptotics [8]:

$$f(E, r) \underset{E \to \infty}{=} \exp(ikr), \qquad k = E^{1/2}.$$

As $f^0(E, r)$ is also an analytical function in the complex plane E with the cut $[0, \infty)$, having no roots and coinciding with $\exp(ikr)$ at large E, the function $\ln F(E, r) = \ln(f(E, r)/f^0(E, r))$ is an analytical function in the E-plane with the cuts $[0, \infty)$, $[E_n(r), -i\infty)$, $n = 1, 2, \ldots, N(r)$. It vanishes at large E; therefore we have

$$\lim_{R \to \infty} \int_{D_R} \frac{\ln F(\tilde{E}, r)}{\tilde{E} - E}\,d\tilde{E} = 0$$

(D_R being the semicircumference of radius R in the upper half-plane). Starting from

this equality after deformation of path of integration and separation of the real part we obtain, in usual way, the dispersion relation

$$\ln|F(E,r)| = \sum_{j=1}^{N(r)} \ln|1 - E_j(r)/E| + \frac{1}{\pi}\int_0^\infty \frac{\arg F(\tilde{E},r)}{\tilde{E}-E}\,d\tilde{E}, \qquad -\infty < E < \infty. \quad (15)$$

The sum in (15) includes all $N(r)$ bound states which exist at given r in the field $U(x)$ on the interval $[r, \infty)$. It is important that relation (15) is valid not only for $E>0$, but also for $E<0$, including the neighbourhoods of $E=E_n(r)$, where both parts of equality have logarithmic singularities. At $r=0$, $E>0$ (15) coincides with (8).

Let us now write the differential relation between $|F(E,r)|$ and $\arg F(E,r)$ at fixed positive energy. At $E>0$ the functions $f(E,r)$ and $f^*(E,r)$ are two independent solutions of the Schrödinger equation with the Wronskian

$$[f(E,r), f^*(E,r)] = -2i\,|f(E,r)|^2\,\partial[\arg f(E,r)]/\partial r = -2iE^{1/2}.$$

From this formula and the similar equality for $f^0(E,r)$, we obtain the necessry relation

$$\frac{\partial}{\partial r}\arg F(E,r) = E^{1/2}(|f(E,r)|^{-2} - |f^0(E,r)|^{-2})$$

$$= E^{1/2}\,|f^0(E,r)|^{-2}(|F(E,r)|^{-2} - 1). \quad (16)$$

After differentiation of (15) with respect to r and substitution of (16) in the result, we have

$$\frac{\frac{\partial}{\partial r}|F(E,r)|}{|F(E,r)|} = \sum_{j=1}^{N(r)} \frac{E_j'(r)}{E_j(r)-E} + \frac{1}{\pi}\int_0^\infty \frac{(|F(\tilde{E},r)|^{-2}-1)\,\tilde{E}^{1/2}}{|f^0(\tilde{E},r)|^2(\tilde{E}-E)}\,d\tilde{E}. \quad (17)$$

This relation is valid for all real E and contains, in fact, all equations of our method. To obtain them in the explicit form we use (17) as it is for $E>0$ and consider the limit $E \to E_n(r)$ $(n=1, 2, ..., N(r))$ for $E<0$. The expansion of $f'(E,r)/f(E,r)$ as a function of E in the neighbourhood of a pole $E=E_n(r)$ has the form

$$\frac{f'(E,r)}{f(E,r)} = \frac{f'}{\dot{f}(E-E_n)}\left[1 + \left(\frac{\dot{f}'}{f'} - \frac{\ddot{f}}{2\dot{f}}\right)(E-E_n) + \cdots\right], \quad (18)$$

where prime and point denote the partial derivatives with respect to r and to E correspondingly. The functions f', $\dot{f}$, $\dot{f}'$, and $\ddot{f}$ in the right-hand part of (18) are taken at $E=E_n(r)$. After differentiation of the identity $f(E_n(r), r) \equiv 0$ with use of the equality $f''(E_n(r), r) = -[E_n(r) - l(l+1)r^{-2} - U(r)]\,f(E_n(r), r) = 0$, we obtain

$$f'(E,r)/\dot{f}(E,r)|_{E=E_n(r)} = -E_n'(r),$$

$$[\dot{f}'(E,r)/f'(E,r) - \ddot{f}(E,r)/2\dot{f}(E,r)]|_{E=E_n(r)} = E_n''(r)/2[E_n'(r)]^2.$$

Substitution of them is (18) gives

$$\frac{f'(E,r)}{f(E,r)} \underset{E\to E_n(r)}{=} -\frac{E_n'(r)}{E-E_n(r)} - \frac{E_n''(r)}{2E_n'(r)} + O(E-E_n(r)). \tag{19}$$

With the use of (19), we obtain from (17), in the limit $E \to E_n(r)$,

$$-\frac{E_n''(r)}{2E_n'(r)} = \frac{f^{0\prime}(E_n(r),r)}{f^0(E_n(r),r)} + \sum_{j\neq n} \frac{E_j'(r)}{E_j(r)-E_n(r)} + \frac{1}{\pi}\int_0^\infty \frac{(|F(\tilde{E},r)|^{-2}-1)\,\tilde{E}^{1/2}\,d\tilde{E}}{|f^0(\tilde{E},r)|^2(\tilde{E}-E_n(r))}. \tag{20}$$

This equation, jointly with Eq. (17) at $E>0$, composes the main system of equations of our approach. As the scattering data are connected (see Eq. (14)) with the values of the functions $|F(E,r)|$, $E_n(r)$, and $C_n(r)$ at $r=0$, it is convenient to transform Eqs. (17) and (20) to a system (of first order) for these functions with the help of relation (9). Moreover, for the convenience of numerical calculations it is necessary to exclude the singularity of the integrand in Eq. (17). This may be done by subtracting

$$\frac{1}{\pi}(|F(E,r)|^{-2}-1)\,|f^0(E,r)|^{-2}E\int_0^\infty \tilde{E}^{-1/2}(\tilde{E}-E)^{-1}\,d\tilde{E}=0$$

from Eq. (17). As a result we obtain the non-linear system

$$\frac{\partial}{\partial r}\ln|F(E,r)| = \sum_{j=1}^{N(r)} [C_j(r)\,|E_j(r)|^l f^{02}(E_j(r),r)(E_j(r)-E)]^{-1} + \frac{1}{\pi}\int_0^\infty \frac{(|F(\tilde{E},r)|^{-2}-1)\,|f^0(\tilde{E},r)|^{-2}\tilde{E} - (|F(E,r)|^{-2}-1)\,|f^0(E,r)|^{-2}E}{\tilde{E}^{1/2}(\tilde{E}-E)}\,d\tilde{E}, \tag{21}$$

$$\frac{\partial}{\partial r}E_n(r) = C_n^{-1}(r)\,|E_n(r)|^{-l}\,|f^0(E_n(r),r)|^{-2}, \tag{22}$$

$$\frac{\partial}{\partial r}\ln C_n(r) = 2\sum_{j\neq n}[C_j(r)\,|E_j(r)|^l f^{02}(E_j(r),r)(E_j(r)-E_n(r))]^{-1} - \left[\frac{l}{E_n(r)} + \frac{2\dot{f}^0(E_n(r),r)}{f^0(E_n(r),r)}\right] C_n^{-1}(r)\,|E_n(r)|^{-l}\,|f^0(E_n(r),r)|^{-2} + \frac{2}{\pi}\int_0^\infty \frac{(|F(\tilde{E},r)|^{-2}-1)\,\tilde{E}^{1/2}\,d\tilde{E}}{|f^0(\tilde{E},r)|^2(\tilde{E}-E_n(r))}. \tag{23}$$

This is the system of ordinary first-order differential equations in which the unknown functions $|F(E, r)|$, $E_n(r)$, $C_n(r)$ are numbered by the continuous parameter $E>0$ and by the discrete index $n=1, 2, ..., N(r)$. It contains neither the interaction potential nor the scattering data. The problem of finding $|F(E, r)|$, $E_n(r)$, $C_n(r)$ $(0 \leqslant E < \infty)$ for the given scattering data is reduced to the Cauchy problem for the system (21)–(23) with initial conditions (14) at $r=0$. The determination of $U(r)$ when $|F(E, r)|$ is known does not present any difficulties (see Eqs. (24)–(27)). So we see that the inverse scattering problem is reduced, in fact, to the Cauchy problem.

The Cauchy problem for Eqs. (21)–(23) with initial conditions at some point r_0 has a unique solution at $r>r_0$ and an infinite set of solutions at $r<r_0$. Although this fact is natural from the physical point of view—the field $U(x)$ influences on $f(E, r)$ only at $x>r$—it needs, of course, a rigorous proof which is the subject of a special investigation and is not considered in the present paper. For the case when the perurbation theory is applicable, this question is studied in [10].

In the point $r=r_n$ $(n=1, 2, ..., N(r))$, where the nth bound state reaches the boundary of the continuum, $E_n(r)$ and $F(0, r)$ become zero, $C_n(r)$ becomes infinite, and $N(r)$ undergoes the sudden change $N(r-0)-N(r+0)=1$. This presents technical difficulties in the numerical calculations, as the system (21)–(23) contains singularities at $r=r_n$. These difficulties, however, may be overcome by the corresponding analytical approximation in the neighbourhood of $r=r_n$ (see Eqs. (28)–(32)).

When bound states are absent, our system consists of the single equation (21) which does not contain the sum; for $l=0$ it was obtained in [10] and has the simplest form

$$\frac{\partial}{\partial r} \ln |F(E, r)| = \frac{1}{\pi} \int_0^\infty \left(\frac{\tilde{E} |F(\tilde{E}, r)|^{-2} - E |F(E, r)|^{-2}}{\tilde{E} - E} - 1 \right) \frac{d\tilde{E}}{\tilde{E}^{1/2}}.$$

After solution of the Cauchy problem and evaluation of $|F(E, r)|$, one can obtain $U(r)$ from the non-linear Milne equation

$$\frac{\partial^2}{\partial r^2} |f(E, r)| + [E - l(l+1) r^{-2} - U(r)] |f(E, r)| = E |f(E, r)|^{-3}. \tag{24}$$

In practice, however, it may be more convenient to calculate $U(r)$ with the help of the asymptotic formula for $|F(E, r)|$ at $E \to \infty$. If $U(r)$ has a continuous derivative, this formula reads

$$|F_l(E, r)| \underset{E \to \infty}{=} 1 + \frac{U(r)}{4E} z \operatorname{Im} \left[f^0_{l-1}(z) f^0_{l+1}(z) f_l^{0*}(z)/f_l^0(z) \right] + o(E^{-1}). \tag{25}$$

Here the notations with explicit dependence on l are used and the fact that $f_l^0(E, r)$ depends only on the product $E^{1/2}r$ is taken into account:

$$f_l^0(E, r) \equiv f_l^0(z), \qquad z = E^{1/2} r.$$

The asymptotic formula (25) is obtained from the Lippman–Swinger integral equation for $f(E, r)$ [8] with the help of integration by parts. It is uniform in the neighbourhood of $r=0$ ($U(0)$ is supposed to be finite). In this point formula, Eq. (25) gives

$$|F_l(E, 0)| \underset{E \to \infty}{=} 1 + \frac{(2l+1)\, U(0)}{4E} + o(E^{-1}). \tag{26}$$

Far from $r=0$, we have

$$|F_l(E, r)| \underset{E \to \infty}{=} 1 + U(r)/4E + o(E^{-1}). \tag{27}$$

4. Computational Method and Numerical Results

Equations (21)–(23) of our approach on the one hand are exact and on the other hand are well suited to be solved numerically with the help of standard calculation methods developed for the Cauchy problem. To estimate the efficiency of such calculations the algorithm based on Eqs. (21)–(23) was worked out and calculations for some examples have been performed.

The Cauchy problem (21)–(23), (14) was solved by the second-order Runge–Kutta method (the midpoint method [12]) with constant stepsize h_r. In the integrals (21), (23) the substitution of variable $E=k^2$ was made. Numerical integration over k was conducted by the Simpson method with constant stepsize h_k on the interval $[0, k_m]$, where $k_m = h_k N_k$, N_k being the number of steps. At $k > k_m$ the approximation

$$|F(k^2, r)| = 1 + A/k^2 + B/k^4$$

was used, where A and B were determined from the equations

$$|F(k_m^2, r)| = 1 + A/k_m^2 + B/k_m^4,$$
$$|F(k_1^2, r)| = 1 + A/k_1^2 + B/k_1^4, \qquad k_1 = k_m - h_k.$$

Using this approximation, corresponding integrals along $k \in [k_m, \infty)$ were calculated analytically.

In the neighbourhood of the point $r=r_n$, $k=0$, the approximation

$$f(k^2, r) = b(r - r_n) - ik/b, \qquad b = f'(0, r_n) \tag{28}$$

was used. This is a truncated Taylor series; in our examples $f(k^2, r)$ is the analytical function of k at $\operatorname{Im} k > \mu < 0$, therefore the expansion into a power series near $k=0$ is legitimate. In Eq. (28) the relation between partial derivatives with respect to r and to k near $r=r_n$, $k=0$,

$$\frac{\partial f(k^2, r)}{\partial r} \cdot \frac{\partial f(k^2, r)}{\partial k} \underset{\substack{k \to 0 \\ r \to r_n}}{=} -i, \tag{29}$$

is taken into account. This relation follows from the study of the normalization integral for $f(E_n(r), r)$ as $r \to r_n$. Indeed, in accordance with Eq. (11) we have

$$\int_r^\infty f^2(E_n(r), x)\, dx = -f'(E_n(r), r) \cdot \dot{f}(E_n(r), r). \tag{30}$$

On the other hand, it is easy to check, that

$$\int_r^\infty f^2(E, x)\, dx \underset{E \to -0}{=} 1/2(-E)^{1/2} + O(1). \tag{31}$$

From Eqs. (30), (31), and equality $\dot{f} = (1/2k)\, \partial f/\partial k$ we obtain Eq. (29).

The expressions for $E_n(r)$ and $C_n(r)$ in the neighbourhood of $r = r_n$, which follow from Eqs. (28) and (9), read

$$E_n(r) = -b^4(r - r_n)^2, \qquad C_n(r) = \frac{r_n^{2l}}{2b^4[(2l-1)!!]^2(r_n - r)}. \tag{32}$$

Calculation of the potential $U(r)$ was conducted simultaneously with the solution of the Cauchy problem (21)–(23), (14) in accordance with asymptotic formula (25). For $l = 0, 1$ it gives

$$|F_0(E, r)| \underset{E \to \infty}{=} 1 + U(r)/4E \tag{33}$$

$$|F_1(E, r)| \underset{E \to \infty}{=} 1 + \frac{U(r)}{4E} \frac{3 + z^2}{1 + z^2}, \qquad z = E^{1/2} r. \tag{34}$$

The numerical test calculations were performed for such scattering data, for which the solution of the inverse problem, i.e., the potential $U(r)$, was known in analytical form. In the first example the calculations were conducted at $l = 0, 1$ and in the others, only at $l = 0$. The following examples were considered:

1. Bound states are absent ($N = 0$). Jost function modulous has the form

$$|F(E)| = (E + a^2)^{1/2}(E + b^2)^{-1/2}. \tag{35}$$

In this case the solution of the inverse problem is the Bargmann potential,

$$U_1(r) = 2(b^2 - a^2) \frac{b^2 - a^2 - x_l^2 + y_l^2}{(x_l - y_l)^2}, \tag{36}$$

where angular momentum l is arbitrary:

$$x_l = \varphi_l^{0\prime}(-b^2, r)/\varphi_l^0(-b^2, r), \qquad y_l = f_l^{0\prime}(-a^2, r)/f^0(-a^2, r).$$

At $l=0, 1$ these values are given by $(a>0,\ b>0)$

$$x_0 = b \operatorname{cth} br, \qquad y_0 = -a \tag{37}$$

$$x_1 = -\frac{1-br+b^2r^2-\exp(-2br)(1+br+b^2r^2)}{r[1-br-\exp(-2br)(1+br)]}$$
$$y_1 = -\frac{1+ar+a^2r^2}{r(1+ar)}. \tag{38}$$

2. The angular momentum and the number of bound states are equal to zero, $l=0$, $N=0$. The Jost function has a double root at $k=-ia$, $a>0$ and a double pole at $k=-ib$, $b>0$; its modulus is given by

$$|F(E)| = (E+a^2)/(E+b^2). \tag{39}$$

These scattering data correspond to the Bargmann potential [10],

$$U_2(r) = U_0(1-\lambda)^2 \times \frac{\exp(x)(\lambda x-\lambda^2-2\lambda+1)-\exp(-x)(\lambda x-\lambda^2+2\lambda+1)\,\lambda^4+4\lambda^3}{[\exp(x)-\lambda^4\exp(-x)-2\lambda^2x+2\lambda^3-2\lambda]^2},$$
$$x=2br, \qquad \lambda=(a-b)/(a+b), \qquad U_0=U_2(0)=4(a^2-b^2). \tag{40}$$

3. The number of bound states N depends on parameter $s>0$

$$N = \text{INTEGER}\left(\frac{s+1}{2}\right);$$

the Jost function modulus, energy levels, and normalization constants are defined by the formulae $(l=0)$

$$|F(E)| = \frac{\pi(k/sh(\pi k))^{1/2}}{|\Gamma(1/2-s/2+ik/2)\,\Gamma(1+s/2+ik/2)|}, \qquad k=E^{1/2}, \tag{41}$$

$$E_n = -(s+1-2n)^2, \tag{42}$$

$$C_n = \frac{\pi^{1/2}2^{n-3}(n-1)!\,\Gamma(s+1-n)}{(s-2n+1)(2n-1)!!\,\Gamma(s-n+3/2)}, \tag{43}$$

where $\Gamma(x)$ is the gamma-function [11]. The solution of the inverse scattering problem in this case is

$$U_3(r) = -s(s+1)\operatorname{ch}^{-2} r. \tag{44}$$

4. The Jost function modulus is given by $(l=0)$

$$|F(E)| = |{}_2F_1(i(\mu-\nu), 1+i(\mu-\nu), 1-2i\nu; x)|, \tag{45}$$

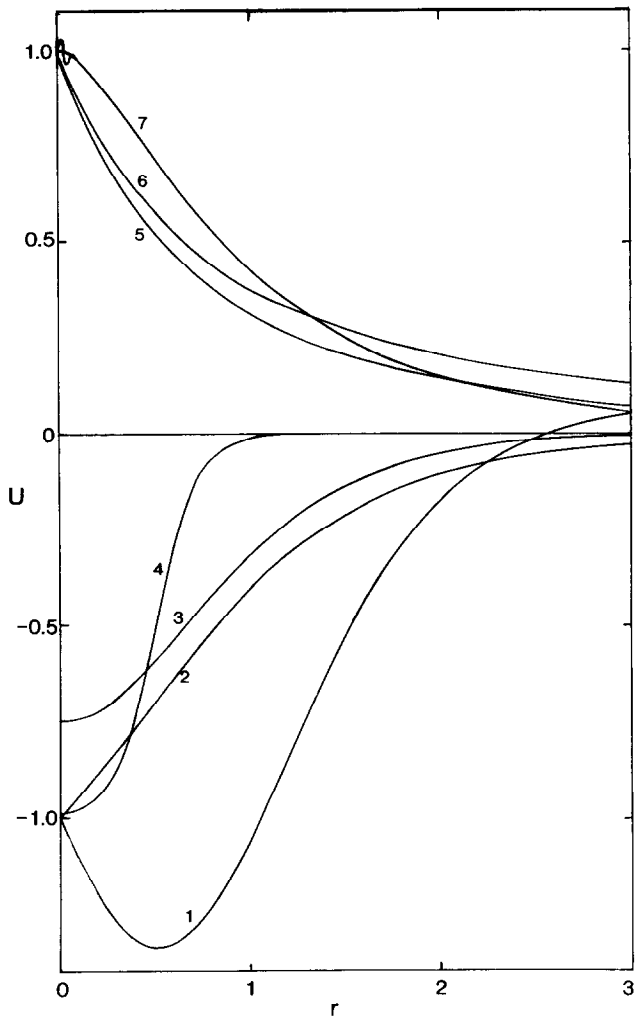

FIG. 1. Some potentials reconstructed by presented method: $U_1(r)$ (Eq. (36))—curves 2 ($l=0$, $U_1(0)=2(a^2-b^2)/(2l+1)=-1.0$, $\lambda=(a-b)/(a+b)=-0.5$); 5 ($l=0$, $U_1(0)=1.0$, $\lambda=0.5$); and 7 ($l=1$, $U_1(0)=1.0$, $\lambda=(7-2\sqrt{10})/3$). $U_2(r)$ (Eq. (40))—curves 1 ($U_2(0)=4(a^2-b^2)=-1.0$, $\lambda=(a-b)/(a+b)=-0.7$) and 6 ($U_2(0)=1.0$, $\lambda=0.5$). $U_3(r)$ (Eq. (44))—curve 3 ($s=0.5$). $U_4(r)$ (Eq. (46))—curve 4 ($U_0=1.0$, $a=0.11$, $R=0.5$). Discrepancy with exact values is visible only for curve 7 (for $l=1$, calculated $U_1(r)$ oscillates at small r).

TABLE I

Potential $U_l(r)$ at $l=0, 1$ for Three Values of the Parameters $U_0 = U_l(0) = 2(a^2-b^2)/(2l+1)$ and $\lambda = (a-b)/(a+b)$

	l	0	0	1
	U_0	−1.0	1.0	1.0
	λ	−0.5	0.5	$(7-2\sqrt{10})/3$
	h_r	0.02	0.02	0.005
	h_k	0.1	0.2	0.4
r	N_k	100	80	100
0.00		−1.00000	1.0000000	1.0000
		−0.99998	0.9999992	0.9991
0.02		−0.98985	0.97064	0.999
		−0.98983	0.97065	1.036
0.04		−0.97942	0.94250	0.996
		−0.97940	0.94253	0.968
0.06		−0.96872	0.91553	0.991
		−0.96870	0.91556	0.983
0.08		−0.95776	0.88965	0.985
		−0.95775	0.88970	0.991
0.10		−0.94657	0.86482	0.9777
		−0.94655	0.86487	0.9776
0.20		−0.88755	0.75442	0.9256
		−0.88754	0.75450	0.9250
0.40		−0.76031	0.58674	0.7874
		−0.76031	0.58684	0.7878
0.60		−0.63180	0.4672	0.64724
		−0.63181	0.4673	0.64726
0.80		−0.51190	0.3791	0.52436
		−0.51192	0.3792	0.52441
1.00		−0.40632	0.3124	0.4225
		−0.40637	0.3125	0.4223
1.20		−0.31730	0.2606	0.3401
		−0.31738	0.2608	0.3397
1.40		−0.24465	0.2197	0.274
		−0.24475	0.2199	0.273
1.60		−0.1868	0.1869	0.222
		−0.1869	0.1871	0.221
1.80		−0.1415	0.1601	0.180
		−0.1417	0.1605	0.179
2.00		−0.1066	0.1381	0.147
		−0.1068	0.1385	0.146
2.20		−0.0800	0.1198	0.120
		−0.0801	0.1202	0.119
2.40		−0.0598	0.1044	0.0989
		−0.0600	0.1048	0.0983
2.60		−0.0446	0.0913	0.0818
		−0.0448	0.0918	0.0816
2.80		−0.0332	0.0802	0.0681
		−0.0333	0.0807	0.0682
3.00		−0.0247	0.0707	0.0570
		−0.0248	0.0712	0.0574
3.20		−0.01837	0.0624	0.0480
		−0.01845	0.0629	0.0486

Note. Upper values are calculated by (36), lower values by our method with scattering data (35). The number of equations N_k and the steps of integration h_r, h_k are also shown.

where ${}_2F_1(\alpha, \beta, \gamma; x)$ is the hypergeometric function [11],

$$v = aE^{1/2}, \qquad \mu = a(E + U_0)^{1/2}, \qquad x = (1 + \exp(-R/a))^{-1}.$$

The values a, R, and U_0 are the parameters. The case without bound states is considered. These scattering data correspond to the Woods–Saxon potential, which is often applied in nuclear physics,

$$U_4(r) = -\frac{U_0}{1 + \exp((r - R)/a)}. \tag{46}$$

The results of the numerical calculations and their comparison with exact values are given in Figs. 1–3 and Tables I–IV.

Figure 1 demonstrates the examples of reconstructed potentials in the absence of bound states. In the figure scale the potentials, obtained by numerical solution of

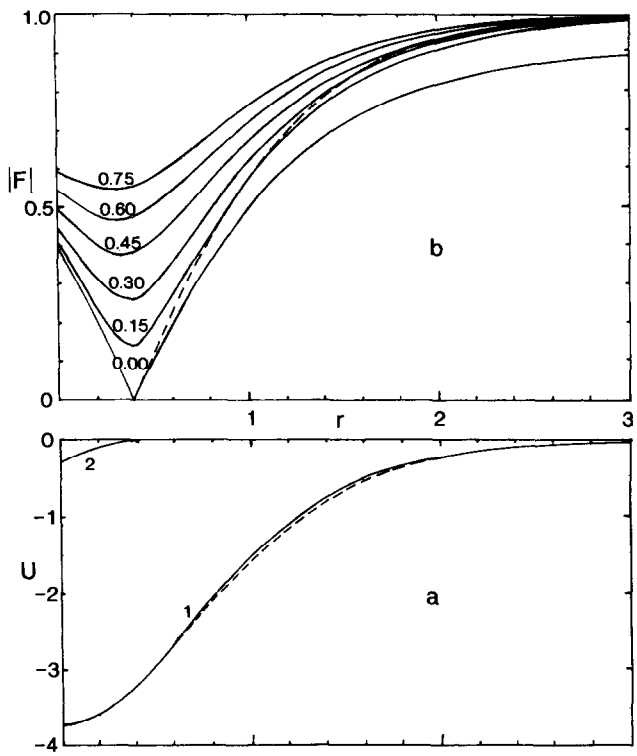

FIG. 2. Reconstruction of potential $U_3(r) = -s(s+1)/ch^2 r$ when one bound state exists ($s = 1.5$): a. Calculated (solid curve 1) and exact (dashed curve 1) values of $U_3(r)$; energy of bound state $E_1(r)$ (curve 2). b. Calculated values of $|F(k^2, r)|$ at $k = 0$, 0.15, 0.30, 0.45, 0.60, 0.75 (solid curves); exact values of $|F(0, r)|$ for $r > r_1$ (dashed curve).

TABLE II

Potential $U_2(r)$ $(l=0)$ for Two Sets of $U_0=4(a^2-b^2)=U_2(0)$ and $\lambda=(a-b)/(a+b)$

	U_0	1.0	−1.0
	λ	0.5	−0.7
	h_r	0.02	0.005
	h_k	0.2	0.05
r	N_k	80	100
0.00		1.000000	−1.000000
		1.000000	−0.999894
0.02		0.974588	−1.024003
		0.974595	−1.024003
0.04		0.95017	−1.04738
		0.95018	−1.04745
0.06		0.92670	−1.0701
		0.92672	−1.0703
0.08		0.90412	−1.0921
		0.90414	−1.0923
0.10		0.88239	−1.1134
		0.88241	−1.1136
0.20		0.78507	−1.207
		0.78510	−1.208
0.40		0.63460	−1.322
		0.63463	−1.323
0.60		0.52491	−1.325
		0.52493	−1.326
0.80		0.44227	−1.224
		0.44230	−1.225
1.00		0.37832	−1.0485
		0.37837	−1.0486
1.20		0.32769	−0.8384
		0.32779	−0.8380
1.40		0.2868	−0.629
		0.2870	−0.628
1.60		0.2533	−0.443
		0.2536	−0.442
1.80		0.2254	−0.292
		0.2258	−0.291
2.00		0.2019	−0.175
		0.2024	−0.174
2.40		0.1647	−0.0307
		0.1654	−0.0301
2.80		0.1367	0.0346
		0.1376	0.0349
3.20		0.1150	0.0572
		0.1160	0.0574
3.60		0.098	0.05959
		0.099	0.05968
4.00		0.084	0.05341
		0.085	0.05342
4.40		0.073	0.04450
		0.074	0.04446

Note. Upper values are calculated by (40), lower values is our result. The parameters h_r, h_k, N_k are also shown.

the inverse problem at $l=0$, coincide with the exact value (36), (40), (44), (46). For $l=1$ the discrepancy is considerable at small r and decreases as r increases (see the last column of Table I).

Figure 2a shows the potential $U_3(r)$ (44) at $s=1.5$, when one bound state exists ($N=1$). Its energy is also shown. The coordinate dependence of $|F(E, r)| = |f(E, r)|$ at different Es, obtained by solution of the Cauchy problem (21)–(23), (14), is presented in Fig. 2b. It is seen that at $E=0$ the discrepancy between calculated and exact $|F(E, r)|$ becomes considerable after the level has merged with the continuum, i.e., at $r \geqslant r_1 = 0.398$. This is probably a consequence of the fact that the approximation we made use of in the vicinity of $r=r_1$ is too rough. The influence of the error in $|F(E, r)|$ at small E on the accuracy of the potential reconstruction is, however, small enough, as it follows from Fig. 2b and from Table III.

Figure 3, taken from [13], is presented for comparison with another method of solution of the inverse problem. It shows the Woods–Saxon potential (46)

TABLE III

Potential $U_3(r)$ ($l=0$) for Different Numbers of Bound States, $N=\text{INTEGER}((s+1)/2)$

	s	0.5	1.5	3.5	19.5
	h_r	0.02	0.02	0.02	0.005
	h_k	0.15	0.15	0.15	0.5
r	N_k	100	120	180	120
0.0		−0.750000	−3.7500	−15.750	−400
		−0.749995	−3.7499	−15.747	−398
0.2		−0.720782	−3.6039	−15.136	−384
		−0.720788	−3.6038	−15.143	−387
0.4		−0.64173	−3.209	−13.48	−342
		−0.64170	−3.202	−13.50	−347
0.6		−0.53368	−2.67	−11.21	−284
		−0.53363	−2.63	−11.21	−291
0.8		−0.41929	−2.10	−8.81	−223
		−0.41924	−2.04	−8.79	−229
1.0		−0.31498	−1.57	−6.62	−168
		−0.31496	−1.52	−6.61	−172
1.4		−0.16211	−0.81	−3.40	−86
		−0.16216	−0.77	−3.39	−91
1.8		−0.07767	−0.39	−1.63	−41
		−0.07772	−0.37	−1.60	−45
2.2		−0.03594	−0.18	−0.75	−19
		−0.03598	−0.17	−0.71	−19
2.6		−0.01637	−0.08	−0.3	−9
		−0.01638	−0.08	−0.7	−6

Note. Upper values are calculated by (44), lower values is our result. The parametrs h_r, h_k, N_k are also shown.

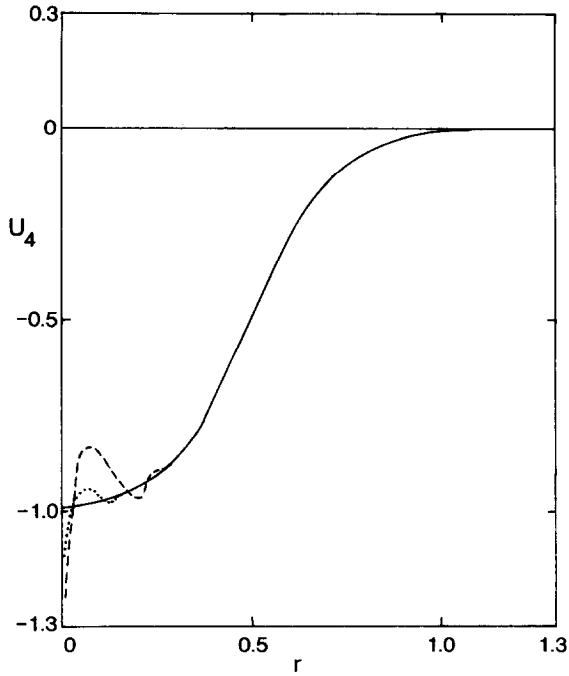

FIG. 3 [13]. Woods–Saxon potential $U_4(r)$ (Eq. (46)) for $U_0 = 1$, $a = 0.11$, $R = 0.5$. Solid line—exact (coincides with calculated in present paper in the figure scale); dashed and dotted lines—calculated in [13] with 4 and 12 adjustable parameters, respectively.

TABLE IV

Woods–Saxon Potential $U_4(r)$ for $U_0 = 1$, $a = 0.11$, $R = 0.5$

r	U	r	U	r	U
0.00	−0.989496	0.08	−0.978505	0.80	−0.061383
	−0.989498		−0.978508		−0.061387
0.01	−0.988508	0.10	−0.974328	0.90	−0.025672
	−0.988509		−0.974333		−0.025680
0.02	−0.987428	0.20	−0.93862	1.00	−0.01050
	−0.987429		−0.93865		−0.01052
0.03	−0.986248	0.30	−0.86035	1.10	−0.00426
	−0.986249		−0.86042		−0.00428
0.04	−0.984959	0.40	−0.71281	1.20	−0.00172
	−0.984960		−0.71285		−0.00175
0.05	−0.983551	0.50	−0.50000	1.30	−0.00069
	−0.983553		−0.49991		−0.00072
0.06	−0.982014	0.60	−0.28719	1.40	−0.00028
	−0.982016		−0.28708		−0.00031
0.07	−0.980336	0.70	−0.13965	1.50	−0.00011
	−0.980338		−0.13962		−0.00014

Note. Upper values are calculated by (46), lower values is our result obtained at $l = 0$, $h_r = 0.005$, $h_k = 0.5$, $N_k = 80$.

reconstructed in the form of the Bargmann potential with n ajustable parameters. It is seen that the error of such a calculation with $n=4$ and with $n=12$ is considerable at small r. The error of our calculation is less than 10^{-4} at all r (see Table IV, and is invisible in this plot.

More complete comparison of calculated and exact values for different potentials is given in Tables I–IV.

The presented results show that using our method one can obtain very high accuracy with the proper choice of h_r, h_k, and N_k. Especially good results are obtained for monotonic potentials at $l=0$, $N=0$. To achieve the same accuracy for non-monotonic potential or in the presence of bound states ($N \geqslant 1$) or in the case $l \geqslant 1$, one must diminish h_r or h_k and increase N_k.

5. Conclusions

The characteristic feature of the proposed approach is that its exact equations are convenient for the direct application of numerical methods. It is achieved due to the transition from the linear equation for a wave function (more exactly, for the Gel'fand–Levitan or Marchenko kernel) to non-linear equations for slowly varying functions having a simple physical meaning. Starting from this idea one can generalize the presented approach to other inverse problems, for example, to the inverse Sturm–Lionville problem and to the inverse scattering problem on the entire real axis. Also it is interesting to develop a similar approach for the inverse scattering problem at fixed energy. As the test calculations give good results even with the simplest computational algorithms we hope that the presented method will be useful for a wide range of problems.

Acknowledgments

The author is grateful to Yu. N. Demkov, V. I. Ochkur, L. I. Ponomarev, and E. A. Solov'ev for stimulating and helpful discussions.

References

1. W. E. Milne, *Phys. Rev.* **35**, 863 (1930).
2. H. J. Korsch, H. Laurent, and R. Mohlenkamp, *J. Phys. B* **15**, 1 (1982).
3. H. J. Korsch and H. Laurent, *J. Phys. B* **14**, 4213 (1981).
4. H. J. Korsch, *Phys. Lett. A* **109**, 313 (1985).
5. B. Yoo and C. H. Greene, *Phys. Rev. A* **34**, 1635 (1986).
6. F. Calogero, *Variable Phase Approach to Potential Scattering* (Academic Press, New York, 1967).
7. V. V. Babikov, *Phase Functions Method in Quantum Mechanics* (Nauka, Moscow, 1968). [Russian]

8. K. CHADAN AND P. C. SABATIER, *Inverse Problems in Quantum Scattering Theory* (Springer-Verlag, New York, 1977).
9. B. M. LEVITAN, *Inverse Sturm–Lionville Problems* (Nauka, Moscow, 1984). [Russian]
10. D. I. ABRAMOV, *Dokl. Akad. Nauk SSSR* **298**, 585 (1988). [Russian]
11. M. ABRAMOWITZ AND I. STEGUN, *Handbook of Mathematical Functions* (Dover, New York, 1968).
12. C. W. GEAR, *Numerical Initial Value Problems in Ordinary Differential Equations* (Prentice–Hall, Englewood Cliffs, NJ, 1971).
13. B. N. ZAKHARYEV, P. YU. NIKISHOV, AND E. B. PLEKHANOV, *Yad. Fiz.* **38**, 95 (1983). [Russian]