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NUMERICAL METHOD FOR SOLVING THE INVERSE PROBLEM OF QUANTUM SCATTERING THEORY

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Численный метод решения обратной задачи
квантовой теории рассеяния

Предложен новый численный метод решения задачи о восстановлении потенциала взаимодействия по фазовому сдвигу, заданному на семействе интервалов в (l,k)-плоскости, удовлетворяющему определенному геометрическому «Условию Лестница». Метод основан на решении уравнения фазовых функций и на модификации непрерывного аналога метода Ньютона.

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Airapetyan R.G., Puzynin I.V., Zhidkov E.P. E11-96-393
Numerical Method for Solving the Inverse Problem
of Quantum Scattering Theory

A new numerical method for solving the problem of the reconstruction of iteraction potential by a phase shift given on a set of closed intervals in (l,k)-plane, satisfying certain geometrical «Staircase Condition», is suggested. The method is based on the Variable Phase Approach and on the modification of the Continuous Analogy of the Newton Method.

The investigation has been performed at the Laboratory of Computing Techniques and Automation, JINR.

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Introduction

The problem of the numerical reconstruction of potential by scattering data is well known and important from the mathematical point of view and for such physical applications as the analysis of a nuclear interaction potential by experimental data. The main approaches for theoretical investigations of the problem are well-known Gelfand-Levitan, Marchenko and Krein methods ([1], [2], [3], [4], [5]). At the same time the development of the corresponding numerical methods is sufficiently complicated by the reason of the ill-posedness of the mentioned inverse problems.

In this paper we consider a new statement of the inverse problem of the Quantum Scattering Theory and suggest the numerical method for its solving. To this end we describe the Newtonian Iterative Scheme with Simultaneous Iterations of the Inverse Derivative and formulate the theorem establishing its convergence. Then we use the method for the inverse problem of the reconstruction of iteraction potential by a phase shift given on a set of closed intervals in (l, k)-plane, satisfying certain geometrical "Staircase Condition".

1. Statement of the Problem

The following Cauchy problem for the radial Schrödinger equation is considered:

$$\frac{\partial^2}{\partial r^2}\phi(l,k,r) + \left(k^2 - \frac{l(l+1)}{r^2}\right)\phi(l,k,r) = V(r)\phi(l,k,r) \qquad (1)$$

$$\lim_{r\to 0}(2l+1)!!r^{-l-1}\phi(l,k,r) = 1 \ . \qquad (2)$$

It is well-known that for the potentials satisfying the condition

$$\int_0^\infty r|V(r)|dr < \infty \qquad (3)$$

the wave function has the following asymptotic behaviour:

$$\phi(l,k,r) \sim \frac{|F(l,k)|}{k^{l+1}}\sin(kr - \frac{\pi l}{2} + \delta(l,k)) \quad r\to\infty \ , \qquad (4)$$

where $F(l,k)$ is the Jost Function.

The Inverse Problem of the Quantum Scattering Theory is the problem of the reconstruction of an unknown potential $V(r)$ by some given information about phase shift $\delta(l,k)$.

Note. For details and complete bibliography we refer to [5], [6], [7], [8], [9].

A potential in (1) is a function of one variable r so it is naturally to reconstruct a potential by a phase shift given on a certain one-dimensional submanifold of (l,k)-plane. The problem is well known and investigated in two important special cases: for the potentials given for fixed orbital momentum l ($\delta(k) = \delta_l(k)$) and for the potentials given for fixed energy (f.i. $\delta(l) = \delta_l(1)$). Geometrically these cases correspond to rays issuing from origin of the (l,k)-plane and parallel to the axes. At the same time there are very few results concerning the potential reconstruction by phase shifts given on another one-dimensional manifolds and all of them are obtained in the framework of the WKB or generalized WKB approaches ([10], [11], [12], [5]). The theoretical analysis of the problem is very difficult because there are no generalization of the Gelfand-Levitan-Marchenko-Krein Theory for such situations.

Our approach to the numerical investigation of these problems is based on the following Variable Phase Equation ([13], [14]):

$$\frac{\partial\delta(l,k,r)}{\partial r} = -k^{-1}V(r)[\cos(\delta(l,k,r))j_l(kr)-$$

$$-\sin(\delta(l,k,r))n_l(kr)]^2, \qquad (5)$$

where

$$\delta(l,k,0) = 0, \quad \lim_{r\to\infty}\delta(l,k,r) = \delta(l,k), \qquad (6)$$

and

$$j_l(z) = \sqrt{\frac{\pi z}{2}}J_{l+1/2}(z), \quad n_l(z) = \sqrt{\frac{\pi z}{2}}Y_{l+1/2}(z) \qquad (7)$$

are Bessel-Ricatti functions.

Let us denote by Φ the nonlinear operator associating to a potential $V(r)$ corresponding phase shift $\delta(l,k)$. Then the inverse problem can be considered as a nonlinear equation

$$\Phi(V) = \delta \qquad (8)$$

with respect to the unknown potential $V(r)$.

2. Continuous Analogy of Newton Method (CANM)

First we describe the Continuous Analogy of Newton Method ([15], [16], [17]).

Let H be a real or complex Hilbert space, $L(H)$ - the space of linear operators in H, $\varphi : H \to H$ - a nonlinear operator. The following nonlinear equation is considered:

$$\varphi(x) = 0 \ . \qquad (9)$$

Denote by x_0 an initial approximation to the solution of the (9), by $\varphi'(x)$ - the Frechét derivative of the operator φ and by $\varphi''(x)$ - the Gateaux derivative of the operator $\varphi'(x)$, i.e. $\varphi''(x)$ for fixed x is a linear operator from H to $L(H)$, such that

$$\varphi'(x+\xi) - \varphi'(x) = \varphi''(x)\xi + \eta, \text{ and } ||\eta||\,||\xi||^{-1} \in 0, \text{ for } \xi \to 0 \ .$$

Now let us consider the following Cauchy problems in H:

$$x'(t) = -\varphi'^{-1}(x(t))\varphi(x(t)), \quad x(0) = x_0 \ . \qquad (10)$$

For the problem the following convergense theorem holds.

Theorem 1. ([15]) *If there exists a positive number r such that the operators $\varphi'(x)$, $\varphi'^{-1}(x)$ and $\varphi''(x)$ exist in any point of the ball $B = \{x; ||x - x_0|| \le r||\varphi(x_0)||\}$, $\varphi''(x)$ is bounded in a neighborhood of every point of B, and for every $x \in B$*

$$||\varphi'^{-1}(x)|| \le r.$$

Then for $t \in [0,+\infty)$ there exists a solution $x(t)$ of the problem (10), $x(t) \in B$ for all $t \in [0,+\infty)$,

$$\lim_{t\in+\infty} x(t) = x^* \qquad (11)$$

and x^* is the solution of the problem (9).

3. The Fréchet Derivative Operator $\Phi'(V)$

So the principal point for solving (8) by means of CANM is the inversion of the operator $\Phi'(V)$. The last one can be simply obtained:

$$(\Phi'(V)\xi)(l,k) = \int_0^\infty K(l,k,t)\xi(t)dt \ , \tag{12}$$

where

$$K(l,k,t) = -B(l,k,t)\exp\Big[\int_t^\infty V(s)A(l,k,s)ds\Big] \ , \tag{13}$$

$$A(l,k,r) = k^{-1}[\sin(2\delta(l,k,r))(j_l^2(kr) - n_l^2(kr))+$$

$$+\cos(2\delta(l,k,r))j_l(kr)n_l(kr)] \ , \tag{14}$$

$$B(l,k,r) = k^{-1}[\cos(\delta(l,k,r))j_l(kr) - \sin(\delta(l,k,r))n_l(kr)]^2 \ . \tag{15}$$

The inversion of the operator (12) is in fact a problem of solving the Fredholm integral equation of first kind. The last one is an ill-posed problem and needs some regularization. In ([18]) the algorithm using Tikhonov regularization at every step of the Newtonian iterations was constructed in the particular case of the problem, when phase shift is given for zero orbital momentum (see also [19]). However such algorithm is unstable and has low accuracy.

Note. For another applications of CANM we refer to [21], [20].

4. Continuous Analogy of Newton Method with the Simultaneous Inversion of the Fréchet Derivative

Now our aim is to consider a continuous Newton method with the simultaneous calculation of reciprocal to the operator $\varphi'(x)$. Let us

consider the following system:

$$\begin{cases} \varphi(x) = 0 \\ \varphi'(x)Y - E = 0 \ , \end{cases} \tag{16}$$

where $Y \in L(H)$ and E is the identity operator. Let Y_0 be some approximation to $\varphi'(x_0)^{-1}$ and ρ is a positive number.

Let us consider the following Cauchy problem:

$$\begin{cases} x'(t) = -Y(t)\varphi(x(t)) \\ Y'(t) = -\rho^2((\varphi'(x(t))^*\varphi'(x(t))Y(t)+ \\ +Y(t)\varphi'(x(t))(\varphi'(x(t)))^*) + 2\rho^2(\varphi'(x(t)))^* \end{cases} \tag{17}$$

$$x(0) = x_0, \quad Y(0) = Y_0 \ .$$

Let us assume that the following condition holds.

Condition A. *There exist $r > 0$ and $\epsilon > 0$ such that*

1) Frechét derivative $\varphi'(x)$ and Gateaux derivative $\varphi''(x)$ exist in $B = B(x_0, r||\varphi(x_0)||)$, moreover

$$||\varphi''||_r = \sup_{x\in B}\ \sup_{\xi\in H, ||\xi||=1} ||(\varphi''(x)\xi||_{L(H)} < \infty \ ,$$

2) for any $x \in B$ the operator $(\varphi'^*(x))$ is invertible and

$$||\varphi'^{*-1}||_r = \sup_{x\in B} ||(\varphi'^*(x))^{-1}|| < \infty \ ,$$

3) the following inequality holds

$$0 < \frac{\max\{||Y_0||, ||\varphi'^{*-1}||_r\}}{1-\max\{||\varphi'(x_0)Y_0 - E||, \epsilon\}} < r \ . \tag{18}$$

Denote

$$||\varphi||_r = \sup_{x\in B} ||\varphi(x)||$$

$$\rho_0 = \max\{||Y_0||, ||\varphi'^{*-1}||_r\}\, ||\varphi'^{-1}||_r \sqrt{\frac{||\varphi''||_r ||\varphi||_r}{2\epsilon}} \ . \tag{19}$$

The following theorem establishes the convergense of the method.

Theorem 2. ([22]) *If the Condition A holds, then for every* $\rho > \rho_0$

1) the solution $(x(t), Y(t))$ *of the problem (17) exists for* $t \in [0, +\infty)$ *and*

$$x(t) \in B(x_0, r||\varphi(x_0)||) \ , \tag{20}$$

$$||\varphi'(x(t))Y(t) - E|| \le \max\{||\varphi'(x_0)Y_0 - E||, \epsilon\} \ ; \tag{21}$$

2) there exists

$$\lim_{t \in +\infty} x(t) = x^*$$

and x^* *is the solution of the problem (9).*

5. An Inversion of the Operator $\Phi'(0)$

So for the numerical solving of the inverse problem by means of the described method we must invert $\Phi'(V)$ only in the initial approximation point $V_0(r)$. As an initial approximation we use zero potential: $V_0(r) \equiv 0$. So we have to solve the following Fredholm equation of first kind:

$$(\Phi'(0)\xi)(l,k) = -\frac{1}{k}\int_0^\infty j_l^2(kr)\xi(r)dr = g(l,k) \ . \tag{22}$$

In the case $l = 0$, $g = g(k)$, $k \in [0, \infty)$ the operator $\Phi'(0)$ is very simple:

$$(\Phi'(0)\xi)(k) = -\frac{1}{k}\int_0^\infty \sin^2(kr)\xi(r)dr \tag{23}$$

and can be easy inversed by means of the Fourier sin-trasformation:

$$(\Phi'(0)^{-1}g)(r) = 2\pi \int_0^\infty \cos(2kr)g(k)kdk \ . \tag{24}$$

Now our goal is to inverse $\Phi'(0)$ for $g(l,k)$ given on more general subset. Let us denote

$$\eta(k) = \int_0^\infty \sin(kr)\xi(r)rdr \ .$$

From the recursion formulas for the Bessel-Ricatty functions

$$\frac{\partial}{\partial x} z_l(x) = \frac{2l+1}{x} z_l(x) - z_{l-1}(x) \quad l = 1, 2, \dots \ ,$$

$$z_{l+1}(x) = z_{l-1}(x) - \frac{l}{x} z_l(x) \quad l = 1, 2, \dots$$

we get the following relations:

$$\frac{\partial}{\partial k}[kg(0,k)] = -\eta(2k) \ , \tag{25}$$

$$\frac{\partial}{\partial k}[kg(l,k)] + \frac{2}{l}g(l,k) = 2\sum_{m=0}^{l-2}(-1)^m(2l-2m-1)g(l-m-1,k) +$$
$$+2(-1)^{l+1}g(0,k) + (-1)^{l+1}\eta(2k) \quad l = 1, 2, \dots \ .$$

Therefore

$$\frac{\partial}{\partial k}[k(g(l,k)+g(l+1,k)] - \alpha_l[k(g(l,k)+g(l+1,k)] = (\beta_l - \alpha_l)g(l+1,k) \ ,$$

$$\frac{\partial}{\partial k}[k(g(l,k)+g(l+1,k)] - \beta_l[k(g(l,k)+g(l+1,k)] = (\alpha_l - \beta_l)g(l,k) \ ,$$

where

$$\alpha_0 = 2, \quad \alpha_l = 2\frac{(l+1)(2l-1)}{l}, \quad \beta_0 = -2, \quad \beta_l = -\frac{2}{(l+1)} \ .$$

So we obtain the following recursions:

$$g(l,k) = a^{1-\alpha_l}[g(l,a) + g(l+1,a)]k^{\alpha_l - 1} +$$
$$+(\beta_l - \alpha_l)k^{\alpha_l - 1}\int_a^k s^{-\alpha_l} g(l+1,s)ds - g(l+1,k) \ , \tag{26}$$

$$g(l+1,k) = a^{1-\beta_l}[g(l,a)+g(l+1,a)]k^{\beta_l-1}+$$

$$+(\alpha_l-\beta_l)k^{\beta_l-1}\int\limits_a^k s^{-\beta_l}g(l,s)ds - g(l,k)\ . \qquad (27)$$

Now let the two finite sequences of nonnegative numbers be given: the first one $\{l_1, l_2, \ldots, l_N\}$ consists of integers, and the second one $\{a_0, a_1, a_2, \ldots, a_{N-1}\}$ of real numbers, where $a_0 = 0$. Denote by I_N a finite set of closed intervals on the (l,k)-plane:

$$I_N = \bigcup_{j=1}^{N-1}\{(l,k); l = l_j, a_{j-1} \le k \le a_j\}\bigcup$$

$$\bigcup\{(l_N,k); a_{N-1} \le k < \infty\}\ . \qquad (28)$$

Definition 1. *We say that the system I_N satisfies a "Staircase Condition" if there exist integers $0 = n_1 < n_2 < \ldots < n_m < N$ such that for every i from 1 to m the following conditions hold*

a) $|l_{j+1} - l_j| = 1$ *for* $j = n_i+1, n_i+2, \ldots, n_{i+1}-1$,

b) no less than one from the numbers $l_{n_i}, l_{n_i+1}, \ldots, l_{n_{i-1}-1}$ *equal to zero.*

From (26) and (27) the following lemma immediatly follows.

Lemma 1. *Let a continuous function* $g(l,k) = \Phi'(0)\xi$ *be given on a set of intervals* I_N *satisfying the "Staircase Condition". Then the corresponding function* $g(0,k)$ *is univalently determined on* $[0,\infty)$ *by recursion formulas (26) and (27).*

From Lemma 1 the recursion formula for the inversion of the operator $\Phi'(0)$ can be easy obtained for every set of intervals satisfying the "Staircase Condition".

6. Statement of the Problem and Numerical Example

Thus, now we can formulate the statement of the problem to which suggested Numerical Method could be applied.

Statement of the Problem. *To reconstruct the potential by means of the phase shift given on the set of the intervals satisfying the "Staircase Condition".*

For this problem there are no theorems establishing its well-posedness, so we are able only to examine it numerically. Let a phase shift $\delta(l,k)$ be given on the set

$$I_2 = \{(1,k); 0 \le k \le a_1\}\bigcup\{(0,k); a_1 \le k \le \infty\}\ . \qquad (29)$$

Then from the formulas of Sect.5 we obtain the following relation:

$$(\Phi'^{-1}(0)g) = \pi(g(0,a)+g(1,a))[(ar^{-1} - \frac{1}{2}a^{-1}r^{-3})\sin(2ar)+$$

$$+r^{-2}\cos(2ar)] + 2\pi\int\limits_a^\infty g(0,k)\cos(2rk)kdk - 2\pi\int\limits_0^a g(1,k)\times$$

$$\times[(k-2k^{-1}r^{-2})\cos(2rk) - (2r^{-1}+k^{-2}r^{-3})\sin(2rk)]dk\ . \qquad (30)$$

Then using this inversion formula for initial approximation we apply the algorithm described in Sect.4.

Below we bring some pictures illustrating the results of the numerical calculations based on this method. We start from the known potential $V_n(r)$ on [0,10], then solve the direct problem and obtain phase shifts $\delta_0(k)$ on [5,10] and $\delta_1(k)$ on [0,5], and finally reconstruct the potential $V_r(r)$ on [0,10].

The results of numerical investigation show that the considered problem can be numerically solved with high accuracy and so such statement of a problem is reasonable. As seems to us, the interesting problem now is to prove the corresponding well-posedness theorem.

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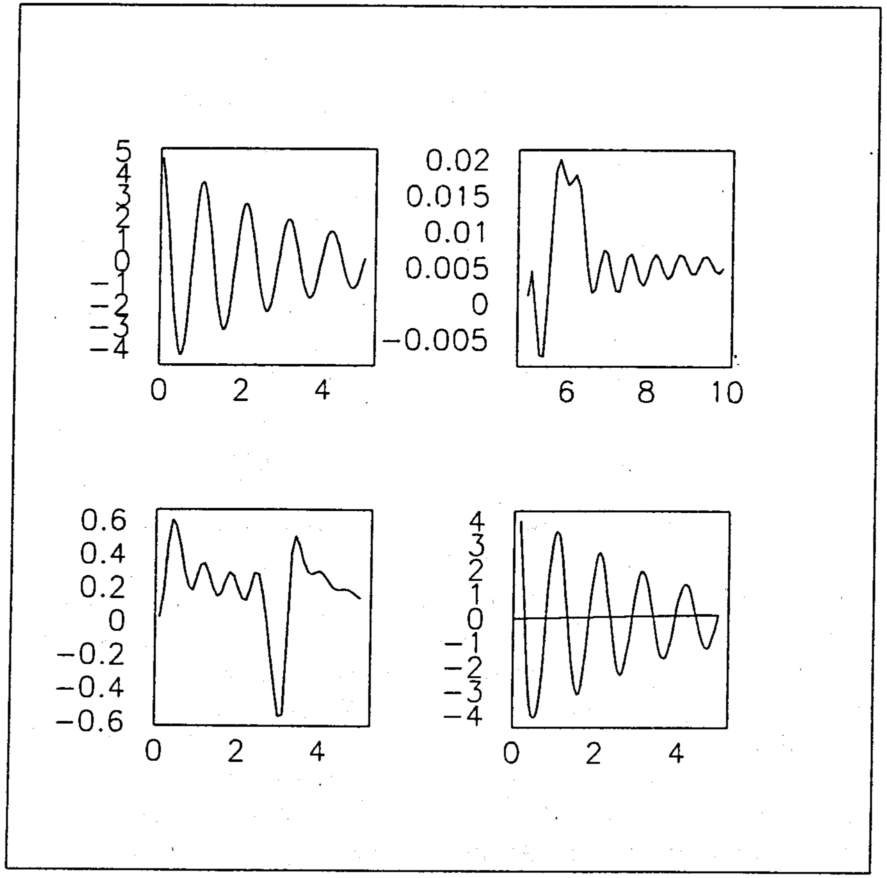

Figure 1: In upper row the first figure displays V_n and second one – δ_0, in lower row the first figure displays δ_1 and second one – V_r.

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