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On a New Statement of Inverse Problem of Quantum Scattering Theory

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Abstract. A new statement of the inverse quantum scattering problem of finding an interaction potential from the given values of phase shift is proposed. The phase shift is given on a set of closed intervals in (l,k)-plane, satisfying certain geometrical "Staircase Condition". For the numerical solution to this problem a new numerical method is described.

1 Introduction

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

$$\frac{\partial^2}{\partial r^2}\phi(l,k,r) + \left(k^2 - \frac{l(l+1)}{r^2}\right)\phi(l,k,r) = V(r)\phi(l,k,r) \tag{1.1}$$

$$\lim_{r\to 0}(2l+1)!!r^{-l-1}\phi(l,k,r) = 1 \quad . \tag{1.2}$$

For potentials from $L_{1,1}(\mathbf{R}_+)$, that is the potentials satisfying the condition

$$||V||_{1,1} = \int_0^\infty r|V(r)|dr < \infty \tag{1.3}$$

the solution to problem (1.1), (1.2) has the following asymptotic behavior:

$$\phi(l,k,r) \sim \frac{|F(l,k)|}{k^{l+1}}\sin(kr - \frac{\pi l}{2} + \delta(l,k)) \quad r\to\infty \ , \tag{1.4}$$

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

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The Inverse Problem of the Quantum Scattering Theory (QST) is a problem of the reconstruction of an unknown potential $V(r)$ from some information about the phase shift $\delta(l,k)$. Because the unknown potential is a function of one variable r and a phase shift is a function of two variables (angular momentum l and energy k), it is natural to state the inverse problem as a problem of finding a potential from the values of the phase shift given a on one-dimensional submanifold of the first quadrant of (l,k)-plane. Indeed in the framework of the known statements of the problem (for fixed angular momentum or fixed energy) the problem of reconstruction of a potential is considered from a phase shift given either on a half-line $\{k \geq 0, l \text{ is fixed}\}$ or on a half-line $\{l \geq 0, k \text{ is fixed}\}$. There are many of books and papers dealing with the theoretical and numerical aspects of these problems (see [**2, 8, 14, 15, 16, 19, 20, 31**]). Detailed bibliography and many applications to physical problems can be found in [**8, 12, 17, 18, 31**]. At the same time there are very few results concerning other statements of the problem. However the analysis of such new statements is interesting for mathematicians and physicists as well. The first question which arises in physical applications of inverse scattering problems is : what kind of scattering information can be used as input ([**17**, p.630]). In [**1, 10**] the inverse problem is investigated for the phase shift given on a continuous curve in (l,k)-plane in the framework of WKB approximation and in [**26, 27**] for the phase shift given on a ray in (l,k)-plane in the framework of generalized Darboux transformations and exactly solvable models. However, because only integer values of an angular momentum have physical meaning the problem of finding a potential by values of the phase shift given for integer values of an angular momentum seems to be of a real physical interest. Below we consider the statement of the problem for the phase shift given for integer values of l and propose numerical method for solution of this problem.

In [**6**] and [**24**] the question of stability of the solution to inverse scattering problem with fixed energy data is investigated. Stability estimates are obtained in [**24**]. A striking uniqueness result is recently obtained in [**21**]. In [**24, 25**] one finds a mathematically justified numerical method for solving 3D inverse scattering problem with fixed energy data. In [**22, 23**] one finds a discussion of the basic results and open problems in the area of multidimensional inverse scattering.

The goal of this work is to describe subsets of (l,k)-plane for which the inverse problem of QST can be solved numerically. To this end we propose a new statement of the inverse problem of the QST for the phase shift given on a set of closed intervals in (l,k)-plane, satisfying the "Staircase Condition". This condition in a weaker form was introduced in [**5**], where also a brief description of the numerical method for solving the inverse scattering problem was given.

Our approach to the solution of the problem is based on the Modification of Continuous Newton Method (MCNM) proposed in [**3**] and [**4**] and on the method of solution of the direct problem of the QST based on the Variable Phase Equation ([**9, 11**]). In this approach we consider the problem as a nonlinear equation $\Phi(V) = 0$ and use MCNM. Unlike in the usual Newton-like methods in the framework of MCNM one is not required to invert the Fréchet derivative operator Φ' at every step of iterations. Instead of this one has to to invert the Fréchet derivative operator $\Phi'(V)$ only at the initial approximation point (in our case $V \equiv 0$). Practically, a high accuracy of the inversion of the Fréchet derivative operator at the initial approximation point is crucial for a successful realization of MNCM. If $[\Phi'(V)]^{-1}$ is found at the initial approximation point $V \equiv 0$, then a specially chosen system of differential equations in Hilbert space realizes the iterative process with the simultaneous calculation of the inverse derivative operator at every step of iterations.

For convenience of the reader in Sect. 2 we briefly repeat the derivation of Variable Phase Equation ([**9**]). It is well known that the direct problem of Quantum Scattering is well-posed, however the applicability of the Variable Phase Equation, which is a nonlinear equation, to the solution to the direct problem needs rigorous proof ([**9**], [**11**] are mostly devoted to physical applications of the Variable Phase Equation and do not contain such a proof). By this reason in Sect. 2 we introduce an appropriate functional space for the solutions of Variable Phase Equation, prove the unique solvability of the Cauchy problem in this space and derive estimates for the solution. We also use these estimates in Sect. 3, where we derive the Fréchet derivative operator $\Phi'(V)$. In Sect. 4 we solve the problem of the inversion of $\Phi'(0)$. In Sect. 5 we discuss MCNM, the numerical method for the solution to the inverse problem of QST and an example.

2 Variable Phase Equation

Our approach to the numerical investigation of these problems is based on the following Variable Phase Equation ([**9**], [**11**]). According to this approach one is looking for the solution to problem (1.1,1.2) in the following form:

$$\phi(l,k,r) = C(l,k,r)[\cos\delta(l,k,r)\cdot u_l(kr) - \sin\delta(l,k,r)\cdot v_l(kr)],$$

where

$$u_l(z) = \sqrt{\frac{\pi z}{2}}J_{l+1/2}(z), \quad v_l(z) = \sqrt{\frac{\pi z}{2}}Y_{l+1/2}(z)$$

are the Bessel-Riccati functions. As in the variation of parameters method let us impose an additional condition on the derivatives of $\delta(l,k,r)$ and $C(l,k,r)$:

$$\frac{\partial}{\partial r}C(l,k,r)[\cos\delta(l,k,r)\cdot u_l(kr) - \sin\delta(l,k,r)\cdot v_l(kr)] =$$

$$= C(l,k,r)\frac{\partial}{\partial r}\delta(l,k,r)[\sin\delta(l,k,r)\cdot u_l(kr) + \cos\delta(l,k,r)\cdot v_l(kr)].$$

Then from (1.1) one has

$$k\frac{\partial}{\partial r}C(l,k,r)[\cos\delta(l,k,r)\cdot u_l'(kr) - \sin\delta(l,k,r)\cdot v_l'(kr)] -$$

$$-kC(l,k,r)\frac{\partial}{\partial r}\delta(l,k,r)[\sin\delta(l,k,r)\cdot u_l'(kr) + \cos\delta(l,k,r)\cdot v_l'(kr)] =$$

$$= V(r)C(l,k,r)[\cos\delta(l,k,r)\cdot u_l(kr) - \sin\delta(l,k,r)\cdot v_l(kr)].$$

Using the following formula for the Wronskian of the functions $u_l(kr)$ and $v_l(kr)$:

$$u_l(kr)\frac{d}{dr}v_l(kr) - v_l(kr)\frac{d}{dr}u_l(kr) = k,$$

and eliminating the derivative $\frac{\partial}{\partial r}C(l,k,r)$, one gets the Variable Phase Equation:

$$\frac{\partial\delta(l,k,r)}{\partial r} = -k^{-1}V(r)[\cos(\delta(l,k,r))u_l(kr) - \sin(\delta(l,k,r))v_l(kr)]^2. \tag{2.1}$$

The solution $\phi(l,k,r)$ should be regular at $r=0$, so

$$\delta(l,k,0)=0. \tag{2.2}$$

From the asymptotic formulas for $u_l(kr)$ and $v_l(kr)$ one obtains that

$$\lim_{r\to\infty}\delta(l,k,r)=\delta(l,k). \tag{2.3}$$

The Variable Phase Equation gives a convenient method for solving the direct problem of quantum scattering theory. However, in order to justify this method one has to prove that problem (2.1), (2.2) is uniquely solvable and that there exists $\lim_{r\to\infty}\delta(l,k,r)$. So first we start with a study of the Cauchy problem (2.1), (2.2). To this end let us define the following Banach space:

$$C_l[0,\infty)=\{u(r): u(r)\in C[0,\infty),$$
$$||u||_l=\sup_{r\in[0,1]}|r^{-2l-1}u(r)|+\sup_{r\in[1,\infty)}|u(r)|<\infty\}.$$

Lemma 2.1 *1. For every $V\in L_{1,1}(\mathbf{R}_+)$ there exists the unique solution $\delta(l,k,r)\in C_l(0,\infty)$ of the problem (2.1), (2.2). 2. There exists finite $\lim_{r\to 0}\delta(l,k,r)$.*

Proof It is assumed in what follows that k is fixed, thus constants below can depend on k. Denote $u(r):=\delta(l,k,r)$, then from (2.1), (2.2) one has

$$u(r)=-\frac{1}{k}\int_0^r V(s)[\cos^2 u(s)u_l^2(ks)-2\sin u(s)\cos u(s)u_l(ks)v_l(ks)+\sin^2 u(s)v_l^2(ks)]ds. \tag{2.4}$$

Let

$$f(r):=-\frac{1}{k}\int_0^r u_l^2(ks)V(s)ds,$$

and

$$A[u](r):=\frac{1}{k}\int_0^r V(s)\sin(u(s))[\sin(u(s))(u_l^2(ks)-v_l^2(ks))+2\cos(u(s))u_l(ks)v_l(ks)]ds, \tag{2.5}$$

then one gets the following nonlinear Volterra equation:

$$u(r)-A[u](r)=f(r). \tag{2.6}$$

Bessel-Riccati functions have the following asymptotics at zero:

$$u_l(r)\sim\frac{\sqrt{\pi}2^{-l-1}}{\Gamma(l+3/2)}r^{l+1},\quad v_l(r)\sim(-1)^{l+1}\frac{\sqrt{\pi}2^l}{\Gamma(-l+1/2)}r^{-l}.$$

Because of the singularity of $v_l(r)$ at $r=0$, first of all one has to prove the unique solvability of (2.6) close to zero.

For some positive number ϵ let us denote by $C_l[0,\epsilon]$ the following Banach space:

$$C_l[0,\epsilon]=\{u(r):u(r)\in C[0,\epsilon],\quad ||u||_{l,\epsilon}=\sup_{r\in[0,\epsilon]}|r^{-2l-1}u(r)|<\infty\}. \tag{2.7}$$

Let f_ϵ be the restriction of f on $[0,\epsilon]$. Since $V(r)\in L_1^1(\mathbf{R}^+)$, one has

$$|f(r)|\le \text{const}\int_0^r s^{2l+2}|V(s)|ds\le \text{const}\cdot r^{2l+1}||V||_{1,1}, \tag{2.8}$$

and one gets that $f_\epsilon\in C_l[0,\epsilon]$. Now our goal is to show that for small enough ϵ the nonlinear operator $A:C_l[0,\epsilon]\to C_l[0,\epsilon]$ is a contraction operator. Indeed, from (2.5) one gets

$$|A[u](r)|\le\frac{1}{k}r^{2l+1}\int_0^r s|V(s)|\cdot|s^{-2l-1}u(s)|\cdot\Bigg(2s^{-1}|u_l(sk)|\cdot|v_l(sk)|+$$

$$+|s^{-2l-1}u(s)|(s^{2l}|u_l(sk)|^2+s^{2l}|v_l(sk)|^2)\Bigg)ds. \tag{2.9}$$

Let us assume that k is fixed and define:

$$c_{1,\epsilon}:=2\sup_{s\in[0,\epsilon]}s^{-1}|u_l(sk)|\cdot|v_l(sk)|,\quad c_{2,\epsilon}:=\sup_{s\in[0,\epsilon]}s^{2l}(|u_l(sk)|^2+|v_l(sk)|^2), \tag{2.10}$$

Then

$$||A(u)||_{l,\epsilon}\le||u||_{l,\epsilon}(c_{1,\epsilon}+c_{2,\epsilon}||u||_{l,\epsilon})\int_0^\epsilon s|V(s)|ds. \tag{2.11}$$

One can choose ϵ such that

$$||f||_{l,\epsilon}(c_{1,\epsilon}+c_{2,\epsilon}||f||_{l,\epsilon})\int_0^\epsilon s|V(s)|ds<1 \tag{2.12}$$

and thus A maps the ball $\{u:u\in C_l[0,\epsilon],\quad ||u||_{l,\epsilon}\le||f||_{l,\epsilon}\}$ into itself. Then

$$A(u^1)-A(u^2)=\frac{1}{k}\int_0^r V(s)\sin(u^1(s)-u^2(s))[\sin(u^1(s)+u^2(s))(u_l^2(ks)-v_l^2(ks))$$

$$+2\cos(u^1(s)+u^2(s))u_l(ks)v_l(ks)]ds,$$

and so

$$||A(u^1)-A(u^2)||_{l,\epsilon}\le||u^1-u^2||_{l,\epsilon}\frac{1}{k}[c_{1,\epsilon}+c_{2,\epsilon}(||u^1||_{l,\epsilon}+||u^2||_{l,\epsilon})]\int_0^\epsilon s|V(s)|ds. \tag{2.13}$$

Thus for small enough ϵ the restriction of A on the ball $\{u:u\in C_l[0,\epsilon],\quad ||u||_{l,\epsilon}\le||f||_{l,\epsilon}\}$ is a contraction operator. This proves the existence and the uniqueness of the solution to problem (2.1), (2.2) on $[0,\epsilon]$. On $[\epsilon,\infty)$ the problem is uniquely solvable because the right hand side of equation (2.1) is majorized by const $\cdot\, V(r)$.

Now one can show that, for $V \in L_{1,1}(\mathbf{R}_+)$, there exists the finite limit

$$\lim_{r\to\infty} u(r) = \int_0^\infty V(s)\sin(u(s))[\sin(u(s))(u_l^2(ks) - v_l^2(ks)) + 2\cos(u(s))u_l(ks)v_l(ks)]ds$$

by using the estimate

$$\int_{R_1}^{R_2} \left| V(s)\sin(u(s))[\sin(u(s))(u_l^2(ks) - v_l^2(ks)) + 2\cos(u(s))u_l(ks)v_l(ks)] \right| ds \le$$

$$\le \text{const} \int_{R_1}^{R_2} |V(s)|ds.$$

□

Denote $B_{1,1}(R) = \{V(r) : V(r) \in L_{1,1}(\mathbf{R}_+) \text{ and } ||V||_{1,1} \le R\}$.

Lemma 2.2 *For the solution $\delta(l,k,r)$ of the problem (2.1), (2.2) with a potential $V(r) \in B_{1,1}(R)$ the following estimate holds:*

$$||\delta(l,k,r)||_l \le c(R) \cdot ||V||_{1,1}, \tag{2.14}$$

where $c(R)$ is some constant depending on R.

Proof From (2.4) one has the following estimate for $r \in [0,\epsilon]$:

$$|r^{-2l-1}u(r)| \le k^{-1}\int_0^r s|V(s)| \cdot (s^{-l-1}|u_l(ks)| + s^{-2l-1}|u(s)| \cdot s^l|v_l(ks)|)^2 ds. \tag{2.15}$$

Thus

$$||u||_{l,\epsilon} \le (c_1 + c_2||u||_{l,\epsilon}) \int_0^\epsilon s|V(s)|ds. \tag{2.16}$$

Let us choose ϵ_R such that

$$c_2 \int_0^{\epsilon_R} s|V(s)|ds < 1,$$

then

$$||u||_{l,\epsilon_R} \le c(R) \cdot ||V||_{1,1}. \tag{2.17}$$

For $r > \epsilon_R$

$$|u(r)| \le |u(\epsilon_R)| + c(R) \cdot \int_{\epsilon_R}^r |V(s)|ds,$$

so

$$\sup_{r \ge \epsilon_R} |u(r)| \le c(R)||V||_{1,1}. \tag{2.18}$$

$\square$

Lemma 2.3 *If $V_1, V_2 \in B_{1,1}(R)$ and $\delta_1(l,k,r)$, $\delta_2(l,k,r)$ are the corresponding solutions of the problem (2.1), (2.2), then the following estimate holds:*

$$||\delta_1(l,k,r) - \delta_2(l,k,r)||_l \le c(R) \cdot ||V_1 - V_2||_{1,1}. \tag{2.19}$$

Proof Denote $u^j(r) := \delta_j(l,k,r)$, $j = 1,2$ and $u = u^1 - u^2$. Then from (2.1) one has

$$u' = -k^{-1} V_1(r)[\cos u^1(r) \cdot u_l(kr) - \sin u^1(r) \cdot v_l(kr)]^2 +$$

$$+ k^{-1} V_2(r)[\cos u^2(r) \cdot u_l(kr) - \sin u^2(r) \cdot v_l(kr)]^2, \quad u(0) = 0. \tag{2.20}$$

Integrating this equation we get the following estimate:

$$|u(r)| \le k^{-1} \int_0^r |V_1(s) - V_2(s)| \cdot [\cos u^1(s) \cdot u_l(ks) - \sin u^1(s) \cdot v_l(ks)]^2 ds +$$

$$+ 2k^{-1} \int_0^r |V_1(s)| \cdot \left| \sin \frac{u^1(s) - u^2(s)}{2} \right| \cdot \left| u_l(ks) \sin \frac{u^1(s) - u^2(s)}{2} + v_l(ks) \cos \frac{u^1(s) + u^2(s)}{2} \right| \cdot$$

$$\cdot \left| u_l(ks)(\cos u^1(s) + \cos u^2(s)) - v_l(ks)(\sin u^1(s) + \sin u^2(s)) \right| ds.$$

Thus we get the estimate

$$|u(r)| \le k^{-1} \int_0^r |V_1(s) - V_2(s)| \cdot [|u_l(ks)| + |u^1(s)| \cdot |v_l(ks)|]^2 ds +$$

$$+ 2k^{-1} \int_0^r |V_1(s)| \cdot |u(s)| \cdot [|u_l(ks)| + |v_l(ks)|] \cdot [|u_l(ks)| + |v_l(ks)|(|u^1(s)| + |u^2(s)|)] ds.$$

For $r < \epsilon_R$

$$|u(r)| \le r^{2l+1} k^{-1} \int_0^r s|V_1(s) - V_2(s)| \cdot [s^{-l-1}|u_l(ks)| + s^{-2l-1}|u^1(s)| \cdot s^l |v_l(ks)|]^2 ds +$$

$$+ 2r^{2l+1} k^{-1} \int_0^r s|V_1(s)| \cdot s^{-2l-1}|u(s)| \cdot s^l [|u_l(ks)| + |v_l(ks)|] \cdot [s^{-l-1}|u_l(ks)| +$$

$$+ s^l |v_l(ks)| \cdot s^{-2l-1}(|u^1(s)| + |u^2(s)|)] ds.$$

Therefore the following estimates follows from Lemma 2.2:

$$r^{-2l-1}|u(r)| \le c_1(R) \int_0^r s|V_1(s) - V_2(s)| ds + c_2(R) \int_0^r s|V_1(s) - V_2(s)| \cdot s^{-2l-1}|u(s)| ds.$$

Now from Gronwall's inequality one gets

$$||u||_{l,\epsilon_R} \leq c(R)||V_1 - V_2||_{1,1} \tag{2.21}$$

For $r \geq \epsilon_R$ it follows from (2.20) that

$$|u(r)| \leq |u(\epsilon_R)| + c_1(r)\int\limits_{\epsilon_R}^{r} |V_1(s) - V_2(s)|ds + c_2(r)\int\limits_{\epsilon_R}^{r} |V_1(s)| \cdot |u(s)|ds.$$

We complete the proof of the Lemma 2.3 using Gronwall's inequality again. □

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

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

$$\Phi(V) = \delta \tag{3.1}$$

with respect to the unknown potential $V(r)$. The principal point for solving (3.1) by means of CNM is the inversion of the operator $\Phi'(V)$.

Lemma 3.1

$$(\Phi'(V)\xi)(l,k) = \int\limits_0^\infty K(l,k,t)\xi(t)dt \ , \tag{3.2}$$

where

$$K(l,k,t) = -B(l,k,t)exp\Big[\int\limits_t^\infty V(s)A(l,k,s)ds\Big] \ , \tag{3.3}$$

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

$$+2\cos(2\delta(l,k,r))u_l(kr)v_l(kr)] \ , \tag{3.4}$$

$$B(l,k,r) = k^{-1}[\cos(\delta(l,k,r))u_l(kr) - \sin(\delta(l,k,r))v_l(kr)]^2 \ . \tag{3.5}$$

Proof Let $\xi(r)$ be an arbitrary function, satisfying condition (1.3) and h be a positive number. Then

$$\Phi(V + h\xi) = \Phi(V) + h\Phi'(V)\xi + o(h).$$

Denote $u(r) := \delta(l,k,r)$ and let $u^h(r)$ be the solution to problem (2.1), (2.2) with a potential $V(r) + h\xi(r)$, so $u^h(0) = u(0)$. From (2.1) one gets

$$\frac{d}{dr}(u^h - u) = -h\xi(r)k^{-1}[\cos u^h(r)\cdot u_l(kr) - \sin u(r)\cdot v_l(kr)]^2 -$$

$$-k^{-1}V(r)[(\cos u^h(r)\cdot u_l(kr) - \sin u^h(r)\cdot v_l(kr))^2 - (\cos u(r)\cdot u_l(kr) - \sin u(r)\cdot v_l(kr))^2].$$

Therefore

$$\frac{d}{dr}(u^h - u) = V(r)A(l,k,r)(u^h - u) - hB(l,k,r)\xi(r) + D(r,h), \tag{3.6}$$

where

$$D(r,h) = 2k^{-1}V(r)(u^h - u)(D_1(r,h) + D_2(r,h) + D_3(r,h)),$$

$$D_1 = \left(\frac{2\sin\frac{u^h-u}{2}}{u^h - u} - 1\right)\cdot\left(u_l(kr)\sin\frac{u^h+u}{2} + v_l(kr)\cos\frac{u^h+u}{2}\right)\cdot$$

$$\cdot\left(u_l(kr)\frac{\cos u^h + \cos u}{2} - v_l(kr)\frac{\sin u^h + \sin u}{2}\right),$$

$$D_2 = \left(u_l(kr)\sin\frac{u^h+u}{2} + v_l(kr)\cos\frac{u^h+u}{2}\right)\cdot\left(u_l(kr)\frac{\cos u^h - \cos u}{2} - v_l(kr)\frac{\sin u^h - \sin u}{2}\right),$$

$$D_3 = \left(u_l(kr)\cos u - v_l(kr)\sin u\right)\cdot\left(u_l(kr)(\sin\frac{u^h+u}{2} - \sin u) + v_l(kr)(\cos\frac{u^h+u}{2} - \cos u)\right).$$

From these expressions one gets the following estimates:

$$|D_i(r,h)| \le \text{const}\cdot r^{-2l}|u^h(r) - u(r)|, \quad i = 1,2,3.$$

So for D one has the following estimate:

$$|D(r,h)| \le \text{const}\cdot r^{-2l}|V(r)|\cdot|u^h(r) - u(r)|^2. \tag{3.7}$$

Since $(u^h - u)(0) = 0$ it follows from (3.6) that:

$$(u^h - u)(r) = -\exp\left[-\int_r^\infty V(s)A(l,k,s)ds\right]\times$$

$$\times\int_0^r \exp\left[\int_t^\infty V(s)A(l,k,s)ds\right](hB(l,k,t)\xi(t) - D(t,h))dt. \tag{3.8}$$

For $r \le 1$

$$|A(l,k,r)| \le k^{-1}r\Bigg(2|r^{-2l-1}u(r)|\cdot(r^{2l}|u_l(kr)|^2 + r^{2l}|u_l(kr)|^2) +$$

$$+2r^{-1}|u_l(kr)|\cdot|v_l(kr)|\Bigg) \le \text{const}\cdot r,$$

and for $r \ge 1$

$$|A(l,k,r)| \le \text{const}.$$

Therefore for any $r \ge 0$

$$\left|\int_r^\infty V(s)A(l,k,s)ds\right| \le c(||V||_{1,1}),$$

where $c(||V||_{1,1})$ is a constant depending on $||V||_{1,1}$. From (3.7)

$$\left|\exp\left[-\int_r^\infty V(s)A(l,k,s)ds\right]\int\limits_0^r \exp\left[\int_t^\infty V(s)A(l,k,s)ds\right]D(t,h)dt\right| \le$$

$$\le c(||V||_{1,1})\left[\int\limits_0^1 t|V(t)|\cdot(t^{-2l-1}|u^h(t)-u(t)|)^2dt + \int\limits_1^\infty |V(t)|\cdot|u^h(t)-u(t)|^2\right] \le$$

$$\le c(||V||_{1,1})\cdot||u^h-u||_l^2 \le h^2c(||V||_{1,1})||\xi(r)||_{1,1}^2,$$

(the last inequality follows from Lemma 2.3). Now let $r\to\infty$, then $u^h - u \to \Phi(V+h\xi) - \Phi(V)$, so one gets:

$$\Phi(V+h\xi)-\Phi(V) = h\int\limits_0^\infty K(l,k,t)\xi(t)dt + O(h^2)$$

where the constant in the asymptotic estimate depends only on $||V(r)||_{1,1}$ and $||\xi(r)||_{1,1}$. Lemma 3.1 is proved. □

4 Inversion of the Operator $\Phi'(0)$

The inversion of the operator (3.2) 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 [**29**] the algorithm using Tikhonov regularization at every step of the Newton's iterations was constructed in the particular case of the problem with zero angular momentum (see also [**30**]). However such algorithm is unstable and has low accuracy.

For the numerical solution of the inverse problem by means of MCNM one should invert $\Phi'(V)$ only in the initial approximation point $V_0(r)$. As an initial approximation we use the potential: $V_0(r)\equiv 0$. So we have to solve the following Fredholm equation of the first kind:

$$(\Phi'(0)\xi)(l,k) = -\frac{1}{k}\int\limits_0^\infty u_l^2(kr)\xi(r)dr \;=\; g(l,k) \quad . \tag{4.1}$$

If $l=0$ and $g=g(0,k)$ is given for all $k\in[0,\infty)$ the operator $\Phi'(0)$ is:

$$(\Phi'(0)\xi)(k) = -\frac{1}{k}\int\limits_0^\infty \sin^2(kr)\xi(r)dr := g(0,k). \tag{4.2}$$

Therefore in this case $\Phi'(0)$ can be easily inverted by means of the Fourier sine-transform:

$$(\Phi'(0)^{-1}g)(r) = \frac{8}{\pi}\int\limits_0^\infty \cos(2kr)g(k)kdk := \Psi_0 g(0,k) \quad . \tag{4.3}$$

For a fixed integer $l \geq 1$ and $g = g(l,k)$ given for $k \in [0,\infty)$ $\Phi'(0)$ can be inverted by means of Mellin transformation M, (see [**7**] or [**18**], p. 318). Indeed

$$\tilde{g}_l(z) := M_{k\to z} g(l,k) = -\frac{1}{k}\int_0^\infty M_{k\to z} u_l^2(kr)\xi(r)dr.$$

Using the formula for Mellin transformation of $J^2_{l+1/2}$ (see [**13**], p. 331) and the relation between u_l and $J_{l+1/2}$ one gets

$$M_{k\to z} u_l^2(kr) = 2^{z-1}\frac{\Gamma(1-z)\Gamma(l+1/2+z/2)}{\Gamma(l+3/2-z/2)\Gamma^2(1-z/2)} r^{-z}, \quad -2l-1 < \Re z < 1.$$

Then from the duplication formula for the gamma function:

$$\Gamma(2z) = \pi^{-1/2}2^{2z-1}\Gamma(z)\Gamma(z+1/2),$$

one obtains the following relation between Mellin images of g and ξ:

$$\tilde{g}_l(z) = b_l(z)\tilde{\xi}(2-z),$$

where

$$b_l(z) = -\frac{\sqrt{\pi}}{4}\frac{\Gamma(1/2-z/2)\Gamma(l+1/2+z/2)}{\Gamma(1-z/2)\Gamma(l-3/2-z/2)}$$

and $\tilde{\xi}(z) = M_{r\to z}\xi$. Therefore

$$\tilde{g}_{l-1}(z) = \frac{l-5/2-z/2}{l-1/2+z/2}\tilde{g}_l(z), \tag{4.4}$$

for $l \geq 1$.

Denote by Ψ_l, $l \geq 1$, the following Mellin pseudodifferential operator of the zero order (for the theory of Mellin pseudodifferential operators see [**28**]):

$$(\Psi_l g)(k) = M^{-1}_{z\to k} a_l(z) M_{s\to z} g(s), \tag{4.5}$$

with the following symbol:

$$a_l(z) = \frac{l-5/2-z/2}{l-1/2+z/2},$$

for $-1 < \Re z < 1$. Thus the following lemma is proved.

Lemma 4.1 *If $l \geq 0$ is fixed and $g(l,k)$ is given on $(0,\infty)$, then one gets the following representation formula for $\Phi'(0)^{-1}$:*

$$\Phi'(0)^{-1} = \Psi_0\Psi_1\ldots\Psi_l. \tag{4.6}$$

Now our goal is to invert $\Phi'(0)$ for $g(l,k)$ given on more general subset. It follows from (4.1) that

$$\frac{\partial}{\partial k}[kg(l,k)] = -2\int_0^\infty u_l'(kr)u_l(kr)\xi(r)rdr. \tag{4.7}$$

From the recursion formulas for the Bessel-Riccati functions (z_l is u_l or v_l)

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

one gets the following relations for $l \geq 2$:

$$\frac{\partial}{\partial k}[kg(l,k)] = \frac{2l}{k} \int\limits_0^\infty u_l^2(kr)\xi(r)dr - 2I_l = -2lg(l,k) - 2I_l,$$

where

$$I_l = \int\limits_0^\infty u_l(kr) j_{l-1}(kr)\xi(r)rdr = \frac{2l-1}{k} \int\limits_0^\infty j_{l-1}^2(kr)\xi(r)dr - I_{l-1}.$$

Since

$$I_{l-1} = -(l-1)g(l-1,k) - \frac{1}{2}\frac{\partial}{\partial k}[kg(l-1,k)],$$

one has the following relation between $g(l,k)$ and $g(l-1,k)$:

$$\frac{\partial}{\partial k}[k(g(l,k) + g(l-1,k))] + 2lg(l,k) - 2lg(l-1,k) = 0. \tag{4.8}$$

For $l = 1$ this formula is also valid, it can be checked easily. Therefore

$$\frac{\partial}{\partial k}[k(g(l,k) + g(l-1,k))] + 2l[g(l,k) + g(l-1,k)] = 4lg(l-1,k) \ ,$$

$$\frac{\partial}{\partial k}[k(g(l,k) + g(l-1,k))] - 2l[g(l,k) + g(l-1,k)] = -4lg(l,k) \ .$$

After the multiplication of this equations by the integrating factor k^{2l} and k^{-2l} respectively and integration from some point a to k one obtains the following recursions:

$$g(l,k) = -g(l-1,k) + a^{2l+1}[g(l,a) + g(l-1,a)]k^{-2l-1} + 4lk^{-2l-1} \int\limits_a^k s^{2l} g(l-1,s)ds, \tag{4.9}$$

$$g(l-1,k) = -g(l,k) + a^{1-2l}[g(l,a) + g(l-1,a)]k^{2l-1} - 4lk^{2l-1} \int\limits_a^k s^{-2l} g(l,s)ds. \tag{4.10}$$

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

$$I_N = \bigcup_{j=1}^{N-1} \{(l,k); l = l_j, a_{j-1} \leq k \leq a_j\} \bigcup \{(l_N,k); a_{N-1} \leq k < \infty\} \ . \tag{4.11}$$

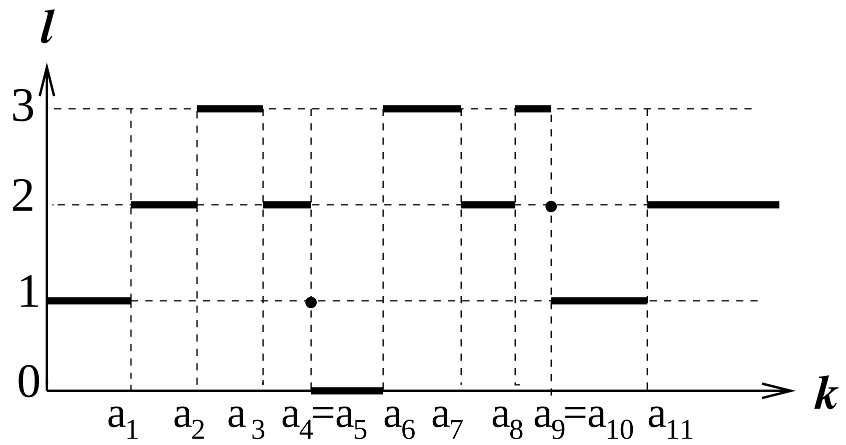

Figure 1 Example of a set satisfying the Staircase Condition (m=2, N=12).

Definition 4.2 We say that the system I_N satisfies a "Staircase Condition" if there exist integers $0 = n_0 < n_1 < \cdots < n_m = N$ such that

a) for every i from 1 to m the following conditions hold

$$|l_{j+1} - l_j| = 1 \text{ for } j = n_{i-1}+1, n_{i-1}+2, \ldots, n_i \quad ,$$

b)

$$\bigcap_{i=1}^{m} \{l_{n_{i-1}+1}, l_{n_i+2}, \ldots, l_{n_i}\} \neq \emptyset \quad . \tag{4.12}$$

From (4.9) and (4.10) the following lemma immediately follows.

Lemma 4.3 *Let a continuous function $g(l,k) = \Phi'(0)\xi$ be given on a set of intervals I_N satisfying the "Staircase Condition". Then for any*

$$l^* \in \bigcap_{i=1}^{m} \{l_{n_{i-1}+1}, l_{n_i+2}, \ldots, l_{n_i}\} \tag{4.13}$$

the corresponding function $g_{l^*}(0,k)$ is uniquely determined on $[0,\infty)$ by recursion formulas (4.9) and (4.10).

From Lemma 4.3 the recursion formula for the inversion of the operator $\Phi'(0)$ can be easily obtained for every set of intervals satisfying the "Staircase Condition". Indeed, one can take any l^* from the intersection (4.13). Then $\Phi'(0)$ can be inverted by means of Lemma 4.1, where $l = l^*$. So the following theorem is proved.

Theorem 4.4 *Let a continuous function $g(l,k)$ be given on a set of intervals I_N satisfying the "Staircase Condition" and assume that $g(l,k)$ belongs to the range of the operator $\Phi'(0)$. Then the equation*

$$\Phi'(0)\xi = g(l,k)$$

has a unique solution, which can be algorithmically computed.

5 Statement of the Problem and Numerical Method

Now we state the problem and describe the numerical method for its solution.

Statement of the Problem. *Given the phase shift on a set of intervals satisfying the "Staircase Condition", find $V(r)$.*

For this problem there are no theorems establishing its well-posedness. We examine this problem numerically. The following approach (MCNM) is used.

Let φ be a nonlinear operator from a Hilbert space H to itself, $L(H)$ be the space of linear operators in H, and A^* be the adjoint of A for any $A \in L(H)$. For solution to nonlinear equation

$$\varphi(x) = 0 \tag{5.1}$$

we consider the following system:

$$\begin{cases} \dot{x}(t) = -Y(t)\varphi(x(t)), \\ \dot{Y}(t) = -\rho^2((\varphi'(x)^*\varphi'(x)Y(t) + Y(t)\varphi'(x)(\varphi'(x))^*) + 2\rho^2(\varphi'(x))^*, \end{cases} \tag{5.2}$$

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

where φ' is the Fréchet derivative of φ, $x(t)$ is a trajectory in H, $Y(t)$ is an operator function from $\mathbf{R}_+$ to $L(H)$, ρ is some positive number, x_0 is an initial approximation point and Y_0 is the inverse operator to $\varphi'(x_0)$. Under certain assumptions on φ and ρ, it is proved in [**3, 4**] that if $t \to +\infty$ then $x(t)$ tends to the solution to problem (5.1).

Explicit formulas (3.2-3.5) and (4.6), (4.9), (4.10) give $\Phi'(V)$ and $[\Phi'(0)]^{-1}$ correspondingly. Thus one can take $x_0 := V_0 \equiv 0$ and $Y_0 = [\Phi'(0)]^{-1}$ as initial data for the Cauchy problem (5.2) and solve problem (5.2) numerically.

Example. Let the phase shift $\delta(l,k)$ be given on the set

$$I_2 = \{(1,k); 0 \le k \le a\} \bigcup \{(0,k); a \le k < \infty\} \ . \tag{5.3}$$

From (4.10)

$$g(0,k) = -g(1,k) + \frac{k}{a}(g(1,a) + g(0,a)) + 4k\int_k^a s^{-2}g(1,s)ds.$$

Since

$$(\Phi'^{-1}(0)g)(r) = \xi(r) = \frac{2}{\pi r}\int_0^\infty \sin(kr)\eta(k)dk,$$

Figure 2 The set in (l,k) - plane, considered in the numerical example.

from (4.6) one gets

$$(\Phi'^{-1}(0)g)(r) = \frac{8}{\pi}\int\limits_0^\infty \cos(2kr)g(0,k)kdk.$$

Thus

$$(Y_0 g)(r) := (\Phi'^{-1}(0)g)(r) = \frac{2}{\pi}\Bigg\{(g(0,a)+g(1,a))[(2ar^{-1} - a^{-1}r^{-3})\sin(2ar)+$$

$$+2r^{-2}\cos(2ar)] + 4\int\limits_a^\infty g(0,k)\cos(2rk)kdk + 4\int\limits_0^a g(1,k)\times$$

$$\times[(2k^{-1}r^{-2} - k)\cos(2rk) + (2r^{-1} - k^{-2}r^{-3})\sin(2rk)]dk\Bigg\}\ . \tag{5.4}$$

This explicit formula defines Y_0, and one can apply MCNM.

One should mention here that the sufficient conditions of convergence theorems for MCNM are much more restrictive than necessary ones. However the numerical applications of the method for solution of nonlinear problems show that very often the method works stably even if the assumptions of convergence theorem are not valid. The results of numerical investigation of the inverse problem (see [**5**]) show that the considered problem can be numerically solved with high accuracy and so such statement of a problem is reasonable. An interesting question now is: is it possible to prove corresponding solvability and uniqueness theorems?

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References

[1] Abramov, D.I. [1984] *On a reconstruction of the interaction potential in semiclassical scattering,* Theor.Mat. Fiz., **58**, 244–253.

[2] Agranovich, Z.S. and Marchenko, V.A. [1960] *Inverse Scattering Problem*, Kharkov.

[3] Airapetyan, R.G. [to appear] *Continuous Newton method and its modification,* Applicable Analysis.

[4] Airapetyan, R.G. and Puzynin, I.V. [1997] *Newtonian iterative scheme with simultaneous iterations of inverse derivative,* Comp. Phys. Comm., **102**, 97-108.

[5] Airapetyan, R.G., Puzynin, I.V. and Zhidkov, E.P. [1997] *Numerical method for solving the inverse problem of quantum scattering theory, (in* [**8**]*)*, Lect. Notes in Phys., **488**, 88-97.

[6] Airapetyan, R.G., Ramm, A.G. and Smirnova, A.B. [1999] *Example of two different potentials which have practically the same fixed-energy phase shifts,* Phys. Lett. A, **254**, issue 3-4, 141-148.

[7] Airapetyan, R.G. and Witt, I. [to appear] *Isometric properties of the Hankel Transformation in Weighted Sobolev Spaces.*

[8] Apagyi, B., Endrédi, G. and Lévay, P. (Eds.), [1997] *Inverse and Algebraic Quantum Scattering Theory, Proceedings, Lake Balaton, Hungary 1996*, Lect. Notes in Phys., **488**, Springer-Verlag, Berlin.

[9] Babikov, V.V. [1968] *The Method of Phase Functions in Quantum Mechanics*, Nauka, Moscow.

[10] Bogdanov, I.V. and Demkov, Yu.N. [1982] *New classical inversion formula for centrally-symmetric electric and magnetic fields and the focusing potentials,* Sov.Phys. JETF, **82**, 1787–1806.

[11] Calogero, F. [1967] *Variable Phase Approach to Potential Scattering,* Academic Press, New York, London.

[12] Chadan, K. and Sabatier, P.C. [1989] *Inverse Problems in Quantum Scattering Theory*, Springer-Verlag.

[13] Erdélyi, A., Magnus, W., Oberhettinger, F. and Tricomi, F.G. [1954] *Tables of Integral Transforms, Vol. I*, McGraw-Hill, New York.

[14] Krein, M.G. [1955] *On a determination of a potential of a particle by its S-function,* DAN SSSR, **105**, 433–436.

[15] Levitan, B.M. [1987] Inverse Sturm-Liouville Problems, VNU Press, Utrecht.

[16] Marchenko, V.A. [1986] *Sturm-Liouville Operators and Applications*, Birkhauser, Basel.

[17] Newton, R.G. [1982] *Scattering Theory of Waves and Particles*, Springer-Verlag.

[18] Ramm, A.G. [1992] *Multidimensional Inverse Scattering Problems*, Longman Group UK Limited, London.

[19] Ramm, A.G. [1988] *Inverse scattering on half-line,* J. Math. Anal. App., **133**, 543-572.

[20] Ramm, A.G. [1998] *A new approach to the inverse scattering and spectral problems for the Sturm-Liouville equation,* Ann. der Phys., **7**, N4, 321-338.

[21] Ramm, A.G. [1999] *Inverse scattering problem with part of the fixed-energy phase shifts,* Comm. Math.Phys.

[22] Ramm, A.G. [1997] *Multidimensional inverse scattering with fixed-energy data,* (in [**8**]), Lect. Notes in Phys., **488**, 373-384.

[23] Ramm, A.G. [1994] *Multidimensional inverse scattering: solved and unsolved problems,* Proc. Intern. Confer. on Dynamical Syst. and Appl., Vol. 1, Atlanta, (Eds. G. Ladde and M. Sambandham), 287–296.

[24] Ramm, A.G. [1992] *Stability estimates in inverse scattering,* Acta Appl. Math., **28**, N1, 1-42.

[25] Ramm, A.G. [1993] *Algorithm for solving 3D inverse scattering problems with noisy discrete fixed-energy data,* Proceedings of ICES-92 conference on inverse problems. In the book: Inverse Problems, Atlanta Technology Publications, Atlanta, Georgia, 70-74.

[26] Schnizer, W.A. and Leeb, H. [1993] *Exactly solvable models for the Schrödinger equation from generalized Darboux transformations,* J. Phys. A: Math. Gen., **26**, 5145-5156.

[27] Schnizer, W.A. and Leeb, H. [1994] *Generalized Darboux transformations: classification of inverse scattering methods for the radial Schrödinger equation,* J. Phys. A: Math. Gen., **27**, 2605-2614.

[28] Schulze, B.-W. [1997] *Boundary Value Problems and Singular Pseudo-Differential Operators,* J. Wiley, Chichester.

[29] Vizner, Ya., Zhidkov, E.P. and Lelek, V. [1968] *The method of a calculation of a potential by means of parameter introduction,* Dubna, JINR, 5-3895.

[30] Vizner, Ya., Zhidkov, E.P., Lelek, V., Malyshev, R.V., Khoromsky, B.N., Hristov, E.H., and Ulegla, I. [1978] *Iterative methods of the solving of an inverse problem of scattering theory,* Part. and Nucl., **9**, 710-768.

[31] Von Geramb, H.V. (Ed.), [1994] *Quantum Inversion Theory and Applications*, Springer-Verlag.