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PIECEWISE-CONSTANT POSITIVE POTENTIALS WITH PRACTICALLY THE SAME FIXED-ENERGY PHASE SHIFTS

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It has recently been shown that spherically symmetric potentials of finite range are uniquely determined by the part of their phase shifts at a fixed energy level $k^2 > 0$. However, numerical experiments show that two quite different potentials can produce almost identical phase shifts. It has been guessed by physicists that such examples are possible only for "less physical" oscillating and changing sign potentials. In this note it is shown that the above guess is incorrect: we give examples of four positive spherically symmetric compactly supported quite different potentials having practically identical phase shifts. The note also describes a hybrid stochastic-deterministic method for global minimization used for the construction of these potentials.

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1. INTRODUCTION

Let $q(x)$, $x \in \mathbb{R}^3$ be a real-valued potential with compact support. Let $R > 0$ be a number such that $q(x) = 0$ for $|x| > R$. We also assume that $q \in L^2(B_R)$, $B_R = \{x : |x| \leq R, x \in \mathbb{R}^3\}$. Let S^2 be the unit sphere, and $\alpha \in S^2$. For a given energy $k > 0$ the scattering solution $\psi(x, \alpha)$ is defined as the solution of

$$(1.1) \quad \Delta\psi + k^2\psi - q(x)\psi = 0, \quad x \in \mathbb{R}^3$$

satisfying the radiation condition

$$(1.2) \quad \lim_{r \rightarrow \infty} \int_{|x|=r} \left| \frac{\partial \psi}{\partial r} - ik\psi \right|^2 ds = 0,$$

where

$$(1.3) \quad \psi = \psi_0 + v, \quad \psi_0 = e^{ik\alpha \cdot x}, \quad \alpha \in S^2.$$

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$$(1.4) \quad \psi(x, \alpha) = \psi_0 + A(\alpha', \alpha, k) \frac{e^{ikr}}{r} + o\left(\frac{1}{r}\right), \text{ as } r \rightarrow \infty, \quad \frac{x}{r} = \alpha'.$$

The function $A(\alpha', \alpha, k)$ is called the scattering amplitude ([7], [8]).

For spherically symmetric scatterers $q(x) = q(r)$ the scattering amplitude satisfies $A(\alpha', \alpha, k) = A(\alpha' \cdot \alpha, k)$. The converse is established in [10]. Following [14], the scattering amplitude for $q = q(r)$ can be written as

$$(1.5) \quad A(\alpha', \alpha, k) = \sum_{l=0}^{\infty} \sum_{m=-l}^l A_l(k) Y_{lm}(\alpha') \overline{Y_{lm}(\alpha)},$$

where Y_{lm} are the spherical harmonics, and the bar denotes the complex conjugate.

The fixed-energy phase shifts $-\pi < \delta_l \leq \pi$ (for this k) are defined ([14]) by the formula:

$$(1.6) \quad A_l(k) = \frac{4\pi}{k} e^{i\delta_l} \sin(\delta_l).$$

Thus, every spherically symmetric potential produces a unique set of phase shifts. The inverse problem of finding the spherically symmetric potential q by the set of its phase shifts has long been of interest in physics. Details and applications can be found in Newton [7] and Chadan-Sabatier [3], where the authors propose a procedure for the identification of the potential q . This procedure has been recently examined by A. G. Ramm. (see [1], part 1).

The following result shows that, theoretically, the inverse problem does have a unique solution given a suitable subset of single-energy phase shifts:

Theorem 1.1 ([9]). *Let $\mathcal{L}$ be an arbitrary fixed subset of non-negative integers satisfying*

$$\sum_{l \in \mathcal{L}, l \neq 0} \frac{1}{l} = \infty.$$

Then the data $\{\delta_l\}_{l \in \mathcal{L}}$, corresponding to a potential $q(r) \in L^2(B_R)$, $R > 0$, $r = |x|$, $q = 0$ for $r > R$, determine $q(r)$ uniquely.

Methods for finding piecewise-constant potentials from fixed-energy shifts were developed in [1], [14], [15]. Numerical results show that, practically, the solution of inverse scattering problem with fixed-energy data can be very unstable towards small perturbation of the data. There exist quite different potentials which produce practically the same phase shifts (at one energy level). The inverse scattering problem with fixed-energy data is ill-posed, see [1] and [15]. After the publication of the example in [1], S. Gutman in [5] has constructed several examples of potentials having practically the same phase shifts, and examined the dependency of the phase shifts on the energy level k . Based on these observations, a best fit to data method involving several energy levels has been proposed and implemented.

However, the potentials in the above examples change sign. Such potentials can be viewed by some physicists as "less physical than one would like to". It has been conjectured by these physicists that it is not possible to construct two different positive potentials which produce practically the same phase shifts at a fixed energy and all angular momenta. AGR has discussed this with Professor W. Scheid (Giessen, Germany). In this note we construct four positive piecewise-constant spherically symmetric potentials having practically identical phase shifts, thus proving that in fact such construction is possible contrary to the belief of some physicists.

Phase shifts and an algorithm for their computation are discussed in Section 2. A hybrid stochastic-deterministic method for finding potentials with practically identical shifts is presented in Section 3. Numerical experiments and the constructed potentials are described in Section 4.

2. PHASE SHIFTS FOR PIECEWISE-CONSTANT POTENTIALS

Below a method from [1] is summarized. Consider a finite set of points $0 = r_0 < r_1 < r_2 < \dots < r_N = R$ and a piecewise-constant potential

$$(2.1) \quad q(r) = q_i, \text{ on } [r_{i-1}, r_i) \text{ for } i = 1, \dots, N, \text{ and } q = 0 \text{ for } r \geq R.$$

Denote $\kappa_i^2 := k^2 - q_i$, where $i = 1, \dots, N$, and k is some fixed positive number. Consider the following problem for the radial Schrödinger equation:

$$(2.2) \quad \frac{d^2 \varphi_l}{dr^2} + \left(k^2 - \frac{l(l+1)}{r^2} \right) \varphi_l = q \varphi_l, \quad \lim_{r \rightarrow 0} (2l+1)!! r^{-l-1} \varphi_l(r) = 1,$$

which we rewrite as:

$$(2.3) \quad \frac{d^2 \varphi_l}{dr^2} + \left(\kappa_i^2 - \frac{l(l+1)}{r^2} \right) \varphi_l = 0$$

on the interval $r_{i-1} \leq r < r_i$. On $[r_{i-1}, r_i)$ one has the following general solution of (2.3)

$$(2.4) \quad \varphi_l(r) = A_i j_l(\kappa_i r) + B_i n_l(\kappa_i r).$$

We assume below that κ_i does not vanish for all i . If $\kappa_i = 0$ for some i then our approach is still valid with obvious changes.

From the regularity of φ_l at zero one gets $B_1 = 0$. Denote $x_i = B_i/A_i$, then $x_1 = 0$. We are looking for the continuously differentiable solution φ_l . Thus, the following interface conditions hold:

$$(2.5) \quad \begin{aligned} A_i j_l(\kappa_i r_i) + B_i n_l(\kappa_i r_i) &= A_{i+1} j_l(\kappa_{i+1} r_i) + B_{i+1} n_l(\kappa_{i+1} r_i), \\ \frac{\kappa_i}{\kappa_{i+1}} [A_i j'_l(\kappa_i r_i) + B_i n'_l(\kappa_i r_i)] &= A_{i+1} j'_l(\kappa_{i+1} r_i) + B_{i+1} n'_l(\kappa_{i+1} r_i). \end{aligned}$$

The Wronskian $W(j_l(r), n_l(r)) = 1$, thus

$$(2.6) \quad \begin{aligned} A_{i+1} &= n'_l(\kappa_{i+1} r_i) [A_i j_l(\kappa_i r_i) + B_i n_l(\kappa_i r_i)] - \frac{\kappa_i}{\kappa_{i+1}} n_l(\kappa_{i+1} r_i) [A_i j'_l(\kappa_i r_i) + B_i n'_l(\kappa_i r_i)], \\ B_{i+1} &= \frac{\kappa_i}{\kappa_{i+1}} j_l(\kappa_{i+1} r_i) [A_i j'_l(\kappa_i r_i) + B_i n'_l(\kappa_i r_i)] - j'_l(\kappa_{i+1} r_i) [A_i j_l(\kappa_i r_i) + B_i n_l(\kappa_i r_i)]. \end{aligned}$$

Therefore

$$(2.7) \quad \begin{pmatrix} A_{i+1} \\ B_{i+1} \end{pmatrix} = \frac{1}{\kappa_{i+1}} \begin{pmatrix} \alpha_{11}^i & \alpha_{12}^i \\ \alpha_{21}^i & \alpha_{22}^i \end{pmatrix} \begin{pmatrix} A_i \\ B_i \end{pmatrix},$$

where the entries of the matrix α^i can be written explicitly:

$$(2.8) \quad \begin{aligned} \alpha_{11}^i &= \kappa_{i+1} j_l(\kappa_i r_i) n'_l(\kappa_{i+1} r_i) - \kappa_i j'_l(\kappa_i r_i) n_l(\kappa_{i+1} r_i), \\ \alpha_{12}^i &= \kappa_{i+1} n_l(\kappa_i r_i) n'_l(\kappa_{i+1} r_i) - \kappa_i n'_l(\kappa_i r_i) n_l(\kappa_{i+1} r_i), \\ \alpha_{21}^i &= \kappa_i j'_l(\kappa_i r_i) j_l(\kappa_{i+1} r_i) - \kappa_{i+1} j_l(\kappa_i r_i) j'_l(\kappa_{i+1} r_i), \\ \alpha_{22}^i &= \kappa_i n'_l(\kappa_i r_i) j_l(\kappa_{i+1} r_i) - \kappa_{i+1} n_l(\kappa_i r_i) j'_l(\kappa_{i+1} r_i). \end{aligned}$$

Thus

$$(2.9) \quad x_{i+1} = \frac{\alpha_{21}^i + \alpha_{22}^i x_i}{\alpha_{11}^i + \alpha_{12}^i x_i}, \quad x_i := \frac{B_i}{A_i}$$

The phase shift $\delta(k, l)$ is defined by

$$(2.10) \quad \varphi_l(r) \sim \frac{|F(k, l)|}{k^{l+1}} \sin(kr - \frac{\pi l}{2} + \delta(k, l)) \quad r \rightarrow \infty ,$$

where $F(k, l)$ is the Jost function. For $r > R$

$$(2.11) \quad \varphi_l(r) = A_{N+1} j_l(kr) + B_{N+1} n_l(kr).$$

From (2.11) and the asymptotics $j_l(kr) \sim \sin(kr - l\pi/2)$, $n_l(kr) \sim -\cos(kr - l\pi/2)$, $r \rightarrow \infty$, one gets:

$$(2.12) \quad \tan \delta(k, l) = -\frac{B_{N+1}}{A_{N+1}} = -x_{N+1} .$$

Finally, the phase shifts of the potential $q(r)$ defined in (2.1) are found from

$$(2.13) \quad \delta(k, l) = -\arctan x_{N+1}.$$

Let $q_0(r)$ be a spherically symmetric piecewise-constant potential. Fix an energy level k and a sufficiently large N . Let $\{\tilde{\delta}(k, l)\}_{l=1}^N$ be the set of its phase shifts. Let $q(r)$ be another such potential, and let $\{\delta(k, l)\}_{l=1}^N$ be the set of its phase shifts.

The best fit to data function $\Phi(q, k)$ is defined by

$$(2.14) \quad \Phi(q, k) = \left(\frac{\sum_{l=1}^N |\delta(k, l) - \tilde{\delta}(k, l)|^2}{\sum_{l=1}^N |\tilde{\delta}(k, l)|^2} \right)^{1/2} ,$$

For sufficiently large N such a function is practically the same as the one which would use all the shifts in (2.14), since the phase shifts are known to decay rapidly with l , see [13]. Our goal is to find positive potentials $q(r)$, quite distinct from $q_0(r)$, that make the objective function small. This is a complex nonlinear minimization problem. An algorithm for its solution is given in the next Section.

3. GLOBAL AND LOCAL MINIMIZATION METHODS

We seek the potentials $q(r)$ in the class of piecewise-constant, spherically symmetric real-valued functions. Let the admissible set be

$$(3.1) \quad A_{adm} \subset \{(r_1, r_2, \dots, r_M, q_1, q_2, \dots, q_M) : 0 \leq r_i \leq R, q_{low} \leq q_m \leq q_{high}\} ,$$

where the bounds q_{low} and q_{high} for the potentials, as well as the bound M on the expected number of layers are assumed to be given.

A configuration $(r_1, r_2, \dots, r_M, q_1, q_2, \dots, q_M)$ corresponds to the potential

$$(3.2) \quad q(r) = q_m, \quad \text{for } r_{m-1} \leq r < r_m, \quad 1 \leq m \leq M ,$$

where $r_0 = 0$ and $q(r) = 0$ for $r \geq r_M = R$.

Note, that the admissible configurations must also satisfy

$$(3.3) \quad r_1 \leq r_2 \leq r_3 \leq \dots \leq r_M .$$

Given an initial configuration $Q_0 \in A_{adm} \subset \mathbb{R}^{2M}$ a local minimization method finds a local minimum near Q_0 . On the other hand, global minimization methods explore the entire admissible set to find a global minimum of the objective function. While the local minimization is usually deterministic, the majority of the global methods are probabilistic in their nature. As usual for these type of inverse problems the best fit to data function Φ has many local minima, see [5]. In this situation it is exceedingly unlikely to get the minima points by chance alone. Thus our special interest is for the minimization methods that combine a global search with a local minimization. In [6] we developed such a method (the Hybrid Stochastic-Deterministic Method), and applied it for the identification of small subsurface particles, given a set of surface measurements. The HSD method could be classified as a variation of a genetic algorithm with a local search with reduction. In [4] two global search algorithms in combination with a special local search method were applied to the identification of piecewise-constant scatterers by acoustic type measurements. The global algorithms considered are the Deep's Method, and Rinnooy Kan and Timmer's Multilevel Single-Linkage Method. The MSLM method has been applied to the identification of piecewise-constant spherically symmetric potentials by their phase shifts in [5].

The potentials in this paper have been found using the so-called Reduced Random Search Method.

In a pure **Random Search** method a batch H of L trial points is generated in A_{adm} using a uniformly distributed random variable. Then a local search is started from each of these L points. A local minimum with the smallest value of Φ is declared to be the global one.

A refinement of the Random Search is the **Reduced Sample Random Search** method. Here we use only a certain fixed fraction $\gamma < 1$ of the original batch of L points to proceed with the local searches. This reduced sample H_{red} of γL points is chosen to contain the points with the smallest γL values of Φ among the original batch. The local searches are started from the points in this reduced sample.

While this method may not be as efficient as the full MSLM algorithm, it has proved to be adequate for the problem at hand.

In our minimization algorithm the Reduced Random Search method is coupled with a deterministic Local Minimization Method.

Numerical experience shows that the objective function Φ is relatively well behaved in this problem. While it contains many local minima and, at some points, Φ is not differentiable, standard minimization methods work well here. A Newton type method for the minimization of Φ is described in [1]. We have chosen to use a variation of Powell's minimization method which does not require the computation of the derivatives of the objective function. Such method needs a minimization routine for a one-dimensional minimization of Φ , which we do using a Bisection or a Golden Rule method. See [4] or [5] for a complete description.

Now we can describe our Basic Local Minimization Method in $\mathbb{R}^{2M}$, which is a modification of Powell's minimization method [2].

Basic Local Minimization Method.

- (1) Initialize the set of directions u_i to the basis vectors

$$u_i = e_i, \quad i = 1, 2, \dots, 2M.$$

- (2) Save your starting position as Q_0 .
- (3) For $i = 1, \dots, 2M$ move from Q_0 along the direction u_i and find the point of minimum Q_i^t .
- (4) Re-index the directions u_i , so that (for the new indices) $\Phi(Q_1^t) \leq \Phi(Q_2^t) \leq \dots, \Phi(Q_{2M}^t) \leq \Phi(Q_0)$.
- (5) For $i = 1, \dots, 2M$ move from Q_{i-1} along the direction u_i and find the point of minimum Q_i .

- (6) Set $v = Q_{2M} - Q_0$.
- (7) Move from Q_0 along the direction v and find the minimum. Call it Q_0 . It replaces Q_0 from step 2.
- (8) Repeat the above steps until a stopping criterion is satisfied.

Note, that we use the temporary points of minima Q_i^t only to rearrange the initial directions u_i in a different order.

Still another refinement of the local phase is necessary to produce a successful minimization. The admissible set A_{adm} , see (3.1)-(3.3), belongs to a $2M$ dimensional minimization space $\mathbb{R}^{2M}$. The dimension $2M$ of this space is chosen a priori to be larger than $2N$, where N is the number of layers in the original potential. We have chosen $M = 6$ in our numerical experiments. However, since the sought potential may have fewer than M layers, we found that conducting searches in lower-dimensional subspaces of $\mathbb{R}^{2M}$ is essential for the local minimization phase. A variation of the following "reduction" procedure has also been found to be necessary in [6] for the search of small subsurface objects, and in [4] for the identification of multilayered scatterers.

If two adjacent layers in a potential have values v_{i-1} and v_i and the objective function Φ is not changed much when both layers are assigned the same value v_i (or v_{i-1}), then these two layers can be replaced with just one occupying their place. The minimization problem becomes constrained to a lower dimensional subspace of $\mathbb{R}^{2M}$ and the local minimization is done in this subspace.

Reduction Procedure. Let ϵ_r be a positive number.

- (1) Save your starting configuration $Q_0 = (r_1, r_2, \dots, r_M, v_1, v_2, \dots, v_M) \in A_{adm}$ and the value $\Phi(Q_0)$. Let the $M + 1$ -st layer be $D_{M+1} = \{r_M \leq |x| \leq R\}$ and $v_{M+1} = 0$.
- (2) For $i = 2, \dots, M + 1$ replace v_{i-1} in the layer D_{i-1} by v_i . Compute Φ at the new configuration Q_i^d , and the difference $c_i^d = |\Phi(Q_0) - \Phi(Q_i^d)|$.
- (3) For $i = 1, \dots, M$ replace v_{i+1} in the layer D_{i+1} by v_i . Compute Φ at the new configuration Q_i^u , and the difference $c_i^u = |\Phi(Q_0) - \Phi(Q_i^u)|$.
- (4) Find the smallest among the numbers c_i^d and c_i^u . If this number is less than $\epsilon_r \Phi(Q_0)$, then adjust the value of the potential to v_i in the "down" or "up" layer accordingly. Replace the two adjacent layers with one occupying their place, and renumber the layers.
- (5) Repeat the above steps until no further reduction in the number of layers is occurring.

Note, that an application of the Reduction Procedure may or may not result in the actual reduction of layers.

Finally, the entire Local Minimization Method (**LMM**) consists of the following:

Local Minimization Method (LMM).

- (1) Let your starting configuration be $Q_0 = (r_1, r_2, \dots, r_M, v_1, v_2, \dots, v_M) \in A_{adm}$.
- (2) Apply the Reduction Procedure to Q_0 , and obtain a reduced configuration Q_0^r containing M^r layers.
- (3) Apply the Basic Minimization Method in $A_{adm} \cap \mathbb{R}^{2M^r}$ with the starting point Q_0^r , and obtain a configuration Q_1 .
- (4) Apply the Reduction Procedure to Q_1 , and obtain a final reduced configuration Q_1^r .

TABLE 1. Phase shifts of $q_0(r)$ for $k = 3$.

l	$\tilde{\delta}(k, l)$	l	$\tilde{\delta}(k, l)$	l	$\tilde{\delta}(k, l)$
0	-0.220024E+00	7	-0.183339E-02	14	-0.204010E-10
1	-0.188623E+00	8	-0.250850E-03	15	-0.766553E-12
2	-0.210693E+00	9	-0.267137E-04	16	-0.253238E-13
3	-0.185306E+00	10	-0.228367E-05	17	-0.741554E-15
4	-0.104318E+00	11	-0.160476E-06	18	-0.193858E-16
5	-0.390310E-01	12	-0.944572E-08	19	-0.455299E-18
6	-0.100159E-01	13	-0.472923E-09	20	-0.966113E-20

4. NUMERICAL RESULTS

Let q_0 be the following potential

$$q_0(r) = \begin{cases} 7.2 & 0 \leq r < 0.5 \\ 4.5 & 0.5 \leq r < 1.0 \\ 7.2 & 1.0 \leq r < 1.5 \\ 4.5 & 1.5 \leq r < 2.0 \\ 0.0 & r \geq 2.0 \end{cases}$$

Let $k = 3$. The phase shifts $\tilde{\delta}(k, l)$ are computed as in Section 2. They are shown in Table 1. Given another piecewise-constant spherically symmetric potential $q(r)$, its phase shifts $\delta(k, l)$ are computed in the same way. The objective function $\Phi(q)$ is formed according to (2.14) with $N = 20$. This objective function is minimized over A_{adm} (3.1) with $M = 6$ and $R = 3.0$ as described in Section 3. A priori bounds for the potential were chosen to be $q_{low} = 0.0$ and $q_{high} = 9.0$. The Reduced Random Search with the batch size $L = 10000$ and the reduction factor $\gamma = 0.01$ was used for the global minimization. The value $\epsilon_r = 0.1$ was used in the Reduction Procedure (see Section 3) during the local minimization phase. The initial configurations were generated using a random number generator with seeds determined by the system time. The run time was about 30 minutes on a 333 MHz PC.

Three potentials with $\Phi(q) < 10^{-4}$ obtained by this procedure are, for example,

$$q_1(r) = \begin{cases} 8.9991 & 0 \leq r < 0.4316 \\ 3.9672 & 0.4316 \leq r < 0.8758 \\ 6.7356 & 0.8758 \leq r < 1.5718 \\ 4.3029 & 1.5718 \leq r < 2.0065 \\ 0.0 & r \geq 2.0065 \end{cases}$$

with $\Phi(q_1) = 9.3586605 \cdot 10^{-5}$,

$$q_2(r) = \begin{cases} 6.4197 & 0 \leq r < 0.6809 \\ 3.1509 & 0.6809 \leq r < 0.9162 \\ 6.7464 & 0.9162 \leq r < 1.2856 \\ 8.7210 & 1.2856 \leq r < 1.4314 \\ 4.5936 & 1.4314 \leq r < 1.9969 \\ 0.0 & r \geq 1.9969 \end{cases}$$

with $\Phi(q_2) = 6.1848208 \cdot 10^{-5}$, and

$$q_3(r) = \begin{cases} 5.9463 & 0 \leq r < 0.8666 \\ 0.1008 & 0.8666 \leq r < 0.9862 \\ 7.9164 & 0.9862 \leq r < 1.4345 \\ 4.6116 & 1.4345 \leq r < 1.9964 \\ 0.0 & r \geq 1.9964 \end{cases}$$

with $\Phi(q_3) = 3.3089927 \cdot 10^{-5}$.

Figures 1, 2 and 3 show these potentials (solid lines) as well as the original potential $q_0(r)$. Potentials q_1 , q_2 and q_3 are quite different from q_0 , but their phase shifts are practically identical to the phase shifts of q_0 . Since real measurements always contain some noise, such a potential is impossible to identify from its phase shifts (at this energy level) by any inverse method.

5. CONCLUSIONS

Recovery of a spherically symmetric potential from its fixed-energy phase shifts is an important physical problem. Recent theoretical results (see Theorem 1.1) assure that such a potential is uniquely defined by a sufficiently large subset of its phase shifts at any one fixed energy level. However, two different potentials can produce almost identical fixed-energy phase shifts. Such examples were obtained in [1] and [5]. These examples give oscillating sign-changing potentials. It was suggested by some physicists that such potentials are "less physical". In this note we present examples of positive spherically symmetric piecewise-constant finite-range potentials having practically the same phase shifts (at a fixed energy level). The existence of such potentials shows that the inverse scattering problem with fixed-energy data can be very ill-posed even if the energy level is not too small. The solution of the inverse scattering problem becomes much more stable if the phase shifts are known at several energy levels, see [5] for details. It is of interest to study the stability of the solution to inverse scattering problem with fixed-energy phase shifts if one assumes a priori that the potential is not only positive but also smooth.

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FIGURE 1. Potential $q_1(r)$ (solid line), and the original potential $q_0(r)$ (dotted line); $\Phi(q_1) = 9.3586605 \cdot 10^{-5}$.

FIGURE 2. Potential $q_2(r)$ (solid line), and the original potential $q_0(r)$ (dotted line); $\Phi(q_2) = 6.1848208 \cdot 10^{-5}$.

FIGURE 3. Potential $q_3(r)$ (solid line), and the original potential $q_0(r)$ (dotted line); $\Phi(q_3) = 3.3089927 \cdot 10^{-5}$.