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# About one numerical algorithm for the solution of the inverse problem with respect to potential

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**Abstract.** In this work the wave equation is analytically solved in the variational form and the analytical expression is found for the gradient of the functional. Also solving the inverse problem with respect to the potential the analytic expression for the optimal potential is obtained. The numerical algorithm for theconsidered problem is given.

Keywords: Inverse problem, variation method, optimal potential

## 1. Introduction

As known, one of the main objectives in theoretical physics since the early years of Quantum Mechanics (QM) is to obtain an exact solution of the wave equation for some special physically important potentials [2,5,9]. Since the wave function contains all necessary information for full description of a quantum system, an analytical solution of the wave equation is of high importance in non-relativistic and relativistic quantum mechanics. Therefore, the analytical and numerical solutions of the Schrodinger equations are of great importance. From this point of view one of serious problems of the applied mathematics, and applied physics are the calculation of energy spectrums and optimal control of their dependence on quantum numbers. Especially in the external magnetic fields, finding the analytical solutions of the wave equations and on the basis of this construction of the optimal solutions depending on quantum numbers is important and interesting [6–8]. There are few potentials for which the wave equation can be solved explicitly for all $n$ and $l$ quantum states [1,11].

The solution of the problem in the studied practical examples appears in various intermediate points of the considered area. The main goal of this problem is finding such potential concerning which the solution of the considered problem would satisfy these conditions. Here the indicated problem is reduced to the variational problem and from this solution the optimality conditions and the formula for the gradient of the functional are found.

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## 2. Problem statement

It is known that the motion of a particle in a central field is described by the following equation

$$-\frac{a}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{bR}{r^2}+q(r)R=ER, \tag{1}$$

here $a > 0$ and $b$ – are given numbers, $q(r)$ – is the energy of interaction. If we multiply the Eq. (1) by the $r^2$ and introduce such substitution

$$Q(r) = b + q(r)r^2,$$

we obtain the following:

$$-a\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+Q(r)R=Er^2R. \tag{2}$$

The analytical solution of the Eq. (2) for different potentials is very interesting. But it is not always possible to obtain the analytical solutions.

In addition, the solution of Eq. (2), finding the potential $Q(r)$ with respect to the energy eigenvalues, i.e., solution of the inverse problem is also very interesting.

Assume that

$$R(r_0) = z_0, R(r_1) = z_1, R(r_2) = z_2, \ldots, R(r_n) = z_n, \tag{3}$$

here

$$0 < r_0 < r_1 < \ldots < r_n; n \geqslant 2.$$

We consider the Eq. (2) on the interval $[r_1, r_n]$. In the work the primary aim is finding the potential $Q(r)$ in the interval $[r_1, r_n]$. We also need to show that the solution of the Eq. (2) $R(r)$ – function satisfies the Eq. (3).

We will assume that the solution of the Eq. (2) is $R(r)$ and the condition $\int_0^\infty R(r)dr < +\infty$ is satisfied. Then the solution of the inverse problem is finding the potential $Q(r)$, which it is necessary that by $r \geqslant 0$, the function $Q(r)$ would be continuously differentiable.

Now we will find the minimum of the following functional

$$J(Q) = \sum_{i=1}^{n-1}[R(r_i) - z_i]^2 \to \min, \tag{4}$$

from the Eq. (2) we obtain the following conditions:

$$R(r_0) = z_0, R(r_n) = z_n. \tag{5}$$

Assume that

$$U = \{Q = Q(r) \in L_2(r_0, r_n) : Q_0 \leqslant Q(r) \leqslant Q_1, \quad \forall r \in [r_0, r_n]\}. \tag{6}$$

Here $0 \leqslant Q_0 < Q_1$ – are given numbers.

We suppose that the function $\psi = \psi(r)$ is solution of the following equation:

$$-a\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right)+Q(r)\psi - Er^2\psi = -2\sum_{i=1}^{n-1}[R(r) - z_i]\delta(r - r_i), \tag{7}$$

$$\psi(r_0) = 0, \psi(r_n) = 0. \tag{8}$$

Applying the traditional technique [3], one can show that the functional Eq. (4) is differentiated and the formula for the gradient

$$J'(Q) = \psi R \tag{9}$$

is true. If $R = R(r)$, $\psi = \psi(r)$, $Q = Q(r)$, then the formulae Eq. (5) is the solution of the Eqs (2), (5), (7) and (8).

## 3. An algorithm for solving the inverse problem

**Algorithm.**

(1) Consider the arbitrary initial potential $Q_0 \leqslant Q(r) \in U$.
(2) Found the solution of the Eqs (2) and (5) with the potential $Q_0(r)$, denote this solution $R_0 = R_0(r)$.
(3) Substituting the solution $R_0 = R_0(r)$ to the sweep problem Eqs (7) and (8), solving this problem we find the function $\psi_0 = \psi_0(r)$.
(4) Using the solutions $R_0 = R_0(r)$ and $\psi_0 = \psi_0(r)$, we found the gradient of the functional Eq. (4).
(5) Minimize the linear functional

$$I_0(Q) = \int_{r_0}^{r_n} \psi_0(r) R_0(r) Q(r) dr \to \min \tag{10}$$

in the set $U$ and find the helper function $\bar{Q}_0 = \bar{Q}_0(r)$.
The new potential is constructed as follows:

$$Q_1(r) = \alpha Q_0(r) + (1-\alpha)\bar{Q}_0(r), \quad 0 \leqslant \alpha \leqslant 1.$$

(6) The accuracy criterion is checked. It may be either such

$$\max_{r_0 \leqslant r \leqslant r_n} |Q_1(r) - Q_0(r)| < \varepsilon,$$

or such $|J(Q_1) - J(Q_0)| < \varepsilon$. In the 6th step the parameter $\alpha$ should be chosen thus that the obtained new values of functional with corresponding $\alpha$ were smaller than previous one

$$J(Q_{k+1}) \leqslant J(Q_k) \text{ or } J(\alpha Q_k + (1-\alpha))\bar{Q}_k \leqslant J(Q).$$

(7) These conditions are called the monotoncity conditions. From the monotoncity conditions can be seen that finding the parameter $\alpha$ from the condition

$$J(\alpha Q_k + (1-\alpha)\bar{Q}_k) \to \min, 0 \leqslant \alpha \leqslant 1$$

is advantaged.

However, finding $\alpha$ from these conditions creates additional difficulties. Therefore it is important to give another method, which is important from a practical point of view.

We assume $\alpha = \frac{1}{2}$ and check the monotoncity condition. If the monotoncity condition is satisfied, then the corresponding $\alpha$ iteration is continued. Otherwise, assuming $\alpha = \frac{1}{4}, \frac{1}{8}, \dots$ the monotoncity condition is checked.

Another way to give iteration formula for each $\alpha$. We can write such as

$$\alpha_k \geqslant 0, \alpha_k \to 0, \sum_{k=1}^{\infty} \alpha_k = \infty.$$

For example we can take $\alpha$ as $\alpha_k = \frac{1}{k+1}$.

Now let's pay attention to the algorithm's doing different operations. As seen from second and third processes in each iteration either basic Eqs (2) and (5) problem or addition Eqs (7) and (8) problems must be solved. It is not always possible to do it on analytic form so it is convenient to do it by the numerical method. If delta function has entered to the Eqs (7) and (8) problems, it solution require special approximation. However for solving problems Eqs (2), (5), (7) and (8) modern programs such as MATLAB can be used.

From the algorithm can be seen that on each $5^{\text{th}}$ step of iteration the linear functional is minimized in the set $U$. The set $U$ has a simple structure and it is solution doesn't create the difficulties. Therefore, the functional Eq. (10) is discredited and is operated within constraints to the linear function of minimization, in other words is reduced to the linear programming problem.

Now let's do one simple problem for demonstration this algorithm.

## 4. Numerical solution

Suppose that the equation

$$-\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+Q(r)R=r^2R, \quad 1\leqslant r\leqslant 3, \tag{11}$$

and the boundary condition

$$R(1)=2, R(3)=10 \tag{12}$$

has been given [4]. It means in this case $\alpha=1$, $E=1$. Our aim is from the set

$$U=\{Q=Q(r)\in L_2(1;3): 2\leqslant Q(r)\leqslant 16\},$$

to find such potential $Q^*=Q^*(r)$, and according to its $R=R(r)$ function, which is the solution of Eqs (11) and (12).

We require the satisfying the condition

$$R(2)=5. \tag{13}$$

It seems that additional condition is just one condition. In variational form we can write it as

$$J(Q)=|R(2)-5|\to\min. \tag{14}$$

If we solve the problems Eqs (11), (12) and (14) by the suggested algorithm method (in this case we use MATLAB), we can find the values for potential

$$R(r)=r^2+1, \tag{15}$$

$$Q^*(r)=\frac{Gr^2}{r^2+1}+r^2. \tag{16}$$

The computing experiment for various values of parameters $N$ and $k$ on the example is carried out. It should be noted that the parameter $N$ shows the splitting number of the difference scheme, and $k$ – the number of iterations. The results of the calculations are given as comparative graphics. The solution of the problem Eqs (11)–(13) is taken as the model problem. We can easily verify that the solution of this problem as follows

$$R(r)=r^2+1,$$

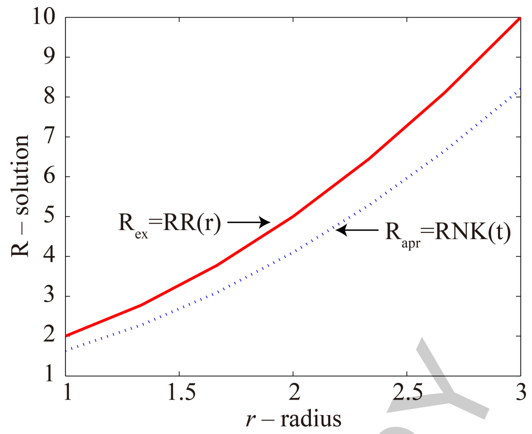


Fig. 1. Identification problem – R solution.

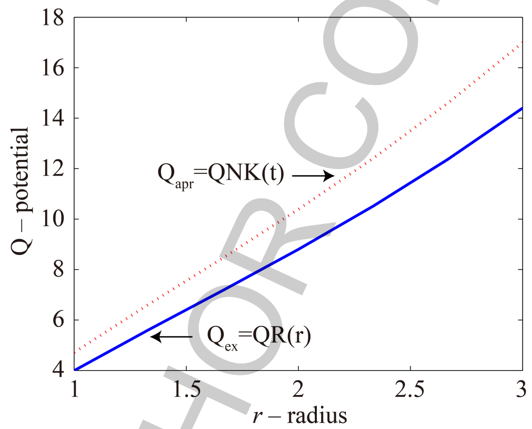


Fig. 2. Identification problem – Q potential.

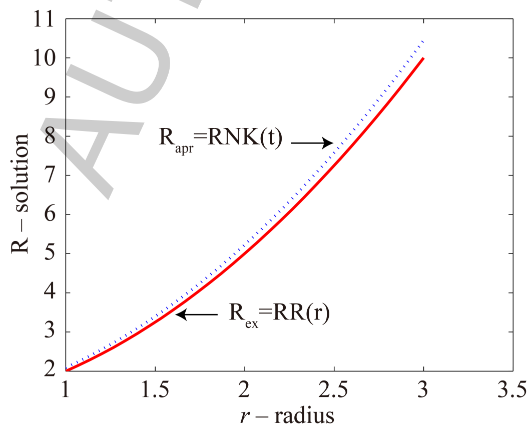


Fig. 3. Identification problem – R solution.

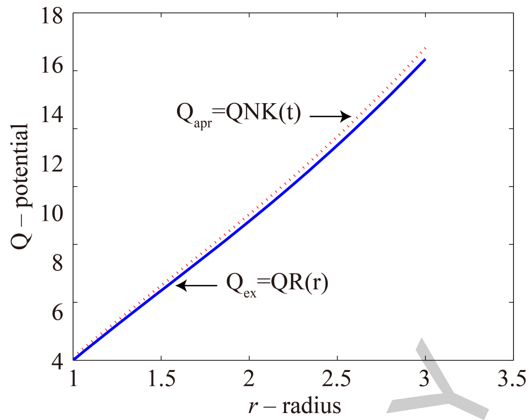


Fig. 4. Identification problem – Q potential.

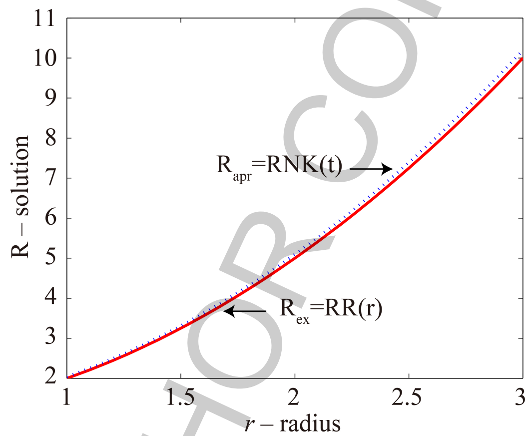


Fig. 5. Identification problem – R solution.

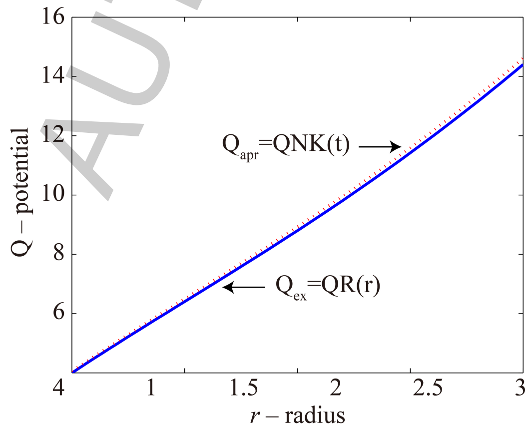


Fig. 6. Identification problem – Q potential.

and the corresponding potential has following form

$$Q*(r) = \frac{Gr^2}{r^2+1} + r^2.$$

In the experiment three cases were considered [10,12]. The solutions and the approximate values of potential were compared with the exact values. The result of the values of parameters $N = 6$, $k = 7$ were given in Fig. 1 ($R$-solution) and Fig. 2 ($Q$-potential) respectively. The graphs show that the approximate solution sufficiently differ from the exact solutions, and therefore they should not be taken as the solution of problem.

Computational experiments carried out for the value $N = 30$, $k = 40$. As can be seen in Figs 3 and 4 the approximate solutions are closer to the exact solution.

At last, in the case $N = 60$, $k = 70$ the results of the calculation show the sufficient accuracy of the realization (Figs 5 and 6).

## 5. Conclusion

The problem of analytical solution of wave equation is reduced to the variational problem one from this solution the optimality conditions and the formula for the gradient of the functional has been is found.

The numerical algorithms for solution of the potential inverse problem have been suggested and the indicated problem has been solved with gradient projection method.



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