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NUMERICAL ALGORITHMS FOR SOLVING THE INVERSE PROBLEM

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

Keywords: Inverse problem, variation method, optimal potential.

AMS Subject Classification: 31A25, 34A55, 65L09.

1. INTRODUCTION

It is known that the motion of a particle in a central field is described by the equation [1-3, 6]

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

Here $a > 0$ and b are given numbers and $q(r)$ is the energy of interaction. Multiplying this equation by the r^2 and denoting

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

we obtain

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

The analytical solution of the equation (2) for different potentials is very interesting. But it is not always possible to obtain the analytical solutions [7].

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

Assume that

$$R(r_0) = z_0, R(r_1) = z_1, R(r_2) = z_2, \dots, R(r_n) = z_n, \quad (3)$$

here

$$0 < r_0 < r_1 < \dots < r_n; \quad n \geq 2.$$

We consider the equation (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 equation (2) $R(r)$ - function satisfies the equation (3).

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

Now we will find the minimum of the following functional

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

from the equation (2) we obtain the following conditions:

$$R(r_0) = z_0, \quad R(r_n) = z_n. \quad (5)$$

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

$$-a \frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) + Q(r)\psi - Er^2\psi = -2 \sum_{i=1}^{n-1} [R(r) - z_i] \delta(r - r_i), \quad (6)$$

Theorem 1. Functional (3) is differentiable and its gradient [8] is given by the formula

$$J'(Q) = \psi R. \quad (7)$$

Theorem 1 allows us to determine the optimal potential analytically.

Theorem 2. Let $Q^* = Q^*(r)$ be the optimal potential for the problem (2),(4), (5). Then for any $Q = Q(r) \subset U$ the relations

$$U = \{Q = Q(r) \in L_2(r_0, r_n) : Q_0 \leq Q(r) \leq Q_1, \quad \forall r \in [r_0, r_n]\}. \quad (8)$$

are true. Here $0 \leq Q_0 < Q_1$ - are given numbers and $R^* = R^*(r), \psi^* = \psi^*(r)$ solutions of a problem (2), (5) at $Q = Q(r)$.

$$\psi(r_0) = 0, \quad \psi(r_n) = 0. \quad (9)$$

2. AN ALGORITHM FOR SOLVING THE INVERSE PROBLEM

1. Consider the arbitrary initial potential $Q_0 \leq Q(r) \in U$.
2. Found the solution of the equations [4, 5] (2), (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 (6),(9), 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 (4).
5. Minimize the linear functional

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

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

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

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

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

or such $|J(Q_1) - J(Q_0)| < \varepsilon$. In the 6th step the parameter α should be chosen thus that the obtained new values of functional with corresponding α were smaller than previous one $J(Q_{k+1}) \leq J(Q_k)$ or $J(\alpha Q_k + (1 - \alpha) \bar{Q}_k) \leq J(Q)$.

These conditions are called the monotonicity conditions. From the monotonicity conditions can be seen that finding the parameter α from the condition

$$J(\alpha Q_k + (1 - \alpha) \bar{Q}_k) \rightarrow \min, \quad 0 \leq \alpha \leq 1$$

is advantaged.

However, finding α 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 monotonicity condition. If the monotonicity condition is satisfied, then the corresponding α iteration is continued. Otherwise, assuming $\alpha = \frac{1}{4}, \frac{1}{8} \dots$ the monotonicity condition is checked.

Another way to give iteration formula for each α . We can write such as

$$\alpha_k \geq 0, \quad \alpha_k \rightarrow 0, \quad \sum_{k=1}^{\infty} \alpha_k = \infty.$$

For example we can take α 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 (2), (5) problem or addition (6), (7) 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 (6), (7) problems, its solution requires special approximation. However for solving problems (2), (5) and (6), (7) modern programs such as MATLAB can be used.

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

3. CONCLUSION

Let $Q^* = Q^*(r)$ by the optimal potential for the problem (2), (3), (4). Then

$$Q^*(r) = \begin{cases} Q_0, & \text{if } \psi^*(r) > 0, \\ Q_1, & \text{if } \psi(r) < 0. \end{cases}$$

In the case $\psi^*(r) = 0$, the potential can be chosen arbitrarily.

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