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Простой метод решения обратной задачи рассеяния

Предлагается новый метод приближенного восстановления по данным рассеяния потенциала в виде кусочно-постоянной ("ступенчатой") функции. Центробежный барьер (при $\ell \neq 0$) и кулоновская компонента взаимодействия могут быть учтены точно. Метод допускает ряд обобщений. Проведены контрольные расчеты.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Melnikov V.N., Rudyak B.V., Zakhariev B.N. **E4 - 10429**

A Simple Method for Solving the Inverse Scattering Problem

A new method of approximate reconstruction of a potential as a step function from scattering data is proposed. The centrifugal barrier (for $\ell \neq 0$) and Coulomb component of interaction can be taken into account exactly. The method admits different generalizations. Numerical calculations for checking the method were performed.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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INTRODUCTION

The reconstruction of a potential from scattering data can be performed by multiple solving the Schroedinger equation (or its analogue, for instance the phase equation) and selecting an appropriate form of potential V(r). That means, the inverse scattering problem is to be solved with the help of the direct one. Recent successful results along this line have been published in [1,2].

In the present paper a more direct way is proposed to determine the shape of a potential from scattering data using the completeness relation of solutions of the Schroedinger equation. It is known that the Parseval equality (the completeness relation) is also necessary to use in order to obtain the basic integral equations of the inverse problem theory (the Gelfand-Levitan-Marchenko equations)* . But in the method suggested in the present paper, the complicated integral equations are not required to be solved.

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* The inverse problem theory has been well developed during the last years (see book [3] and review article [4]).

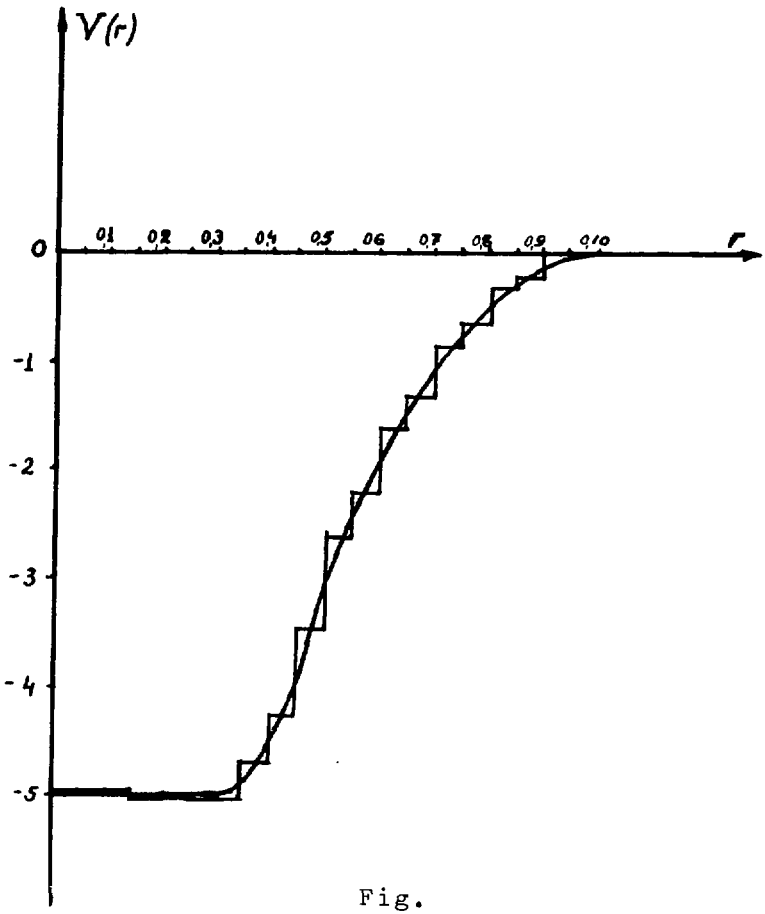

Fig.

The potential V_{step} was reconstructed from 50 pairs of parameters $\{E_\lambda, \gamma_\lambda\}$ the first 13 of which were determined by the solution of the direct problem (with V(r)) and other 37 were taken in quasiclassical approximation (with a single parameter $\int V dr$ taken from asymptotic behaviour of E_λ).

In the proposed algorithm of the inverse problem solution the approximation of potential $V(r)$ by step function $V_{step}(r)$ as is shown in the figure is used.

The advantage of an approximation of this type is a simple analytical solvability of the Schroedinger equation ($\hbar=1$):

$$-\frac{1}{2m}\Psi''(r)+V(r)\Psi(r)=E\Psi(r); \qquad (1)$$

$$\Psi(0)=0,$$

in each interval $[r_i \le r \le r_{i-1}]$ of the coordinate axis, corresponding to one step of V_{step}, where $V_{step}(r)=\text{const}$. So we have:

$$\Psi(E, r_i \le r \le r_{i-1}) = A_i(E)e^{-ik_i r} + B_i(E)e^{ik_i r}; \qquad (2)$$

$$k_i = \sqrt{2m(E-V_i)}. \qquad (2')$$

If the values V_i are known, the direct problem is easily solved (see for example /6/), the coefficients A_i, B_i are determined from the conditions of smooth sewing of wave functions given on neighbouring intervals at the points r_{i-1}.

The solution of the inverse problem is somewhat more complicated because besides A_i, B_i, also the unknown values V_i are to be determined. As the additional relations for determining A_i, B_i, V_i we use the Parseval equality:

$$\sum_n \Psi_n(r)\Psi_n^*(r') + \frac{1}{2\pi}\int_0^\infty \Psi(k,r)\Psi(k,r')dk = \delta(r-r'), \qquad (3)$$

where the asymptotic behaviour of Ψ is determined by (4). The procedure of reconstruction of V_i from the given behaviour of the wave function Ψ outside the interac-

tion region (the scattering phase shift is assumed to be known) is described in sect.2 of this article. The inverse problem formalism is simplified in the framework of the R-matrix scattering theory, where instead of phase shift $\delta(E)$ as a continuous function of energy, the discrete set of constants: R-matrix resonance positions E_λ and their reduced widths γ_λ^2, are used as initial parameters in the inverse problem (sect. 3).

The suggested method allows one to take into account exactly the additional centrifugal barrier for partial waves with angular momentum $\ell > 0$, and also the Coulomb potential.

Instead of simple rectangular steps, the peaces of potentials of another shape for which the analytical solution of the Schroedinger equation is known, can be used to approximate V(r).

Multichannel systems, as for example, the motion of a particle in the field of tensor forces, are described by the system of coupled Schroedinger equations. The inverse problem in this case is the matrix generalization of the single-channel formalism.

The numerical calculations were performed in order to verify the developed method. The regularization following the Tichonov theory[7] was used for stabilizing the algorithm of the potential reconstruction.

2. RECONSTRUCTION OF A POTENTIAL FROM PHASE SHIFTS AND BOUND STATE PARAMETERS

The unknown potential is for simplicity supposed to have a finite range a: $V(r \geq a) = 0$. The wave function Ψ outside the interaction region has the form (we consider at first the case $\ell = 0$)*:

$$\Psi(E, r \geq a) = e^{-ikr} - S(k) e^{ikr}, \quad \text{if } E > 0, \tag{4}$$

$$\Psi(E_n, r \geq a) = C_n e^{-\kappa_n r}, \quad \text{for bound states.} \tag{4'}$$

The quantities $S(k) = e^{2i\delta(k)}$, κ_n, C_n are assumed to be known, and it is required to determine Ψ and V for $r < a$.

From the continuity condition of wave function Ψ and its first derivative Ψ' at point $r = a$, using the expressions for Ψ in the form (4), (4') for $r \geq a$ and (2), (2') for $r_1 \leq r \leq r_0 = a$ we get

$$A_1(E) e^{-ik_1 a} + B_1(E) e^{ik_1 a} = \begin{cases} e^{-ika} - S(k) e^{ika}, & \text{if } E > 0 \\ C_n e^{-\kappa_n a}, & \text{if } E = E_n < 0 \end{cases} \tag{5}$$

$$k_1 [A_1(E) e^{-ik_1 a} - B_1(E) e^{ik_1 a}] = \begin{cases} k [e^{ika} + S(k) e^{ika}], & \text{if } E > 0 \\ \frac{\kappa_n}{i} e^{-\kappa_n a}, & \text{if } E = E_n < 0 \end{cases} \tag{6}$$

The relations (5), (6) can be considered as a system of two linear algebraic equations for the coefficients A_1, B_1. Solving (5), (6), we find, for each value E, these coefficients as functions of the pa-

* For numerical calculations it is convenient to operate with real values and one can take Ψ in the form: $\Psi = A \sin(kr + \delta)$.

rameter V_1. The desired value of V_1 is fixed by the Parseval equality (3) if Ψ in the form (2) with coefficients A (E) and B (E) expressed through V, is substituted into (3). In order to avoid the integration in (3) over the infinite continuous spectrum, the Parseval equality for free waves

$$\frac{2}{\pi}\int_0^\infty \sin kr \sin kr' \, dk = \delta(r-r') \qquad (7)$$

should be subtracted from eq. (3). Taking into account, that for the energy values $E>E_{max}$, which are much larger than the potential absolute values ($E_{max}\gg|V|$), the wave function Ψ is approximately equal to the free wave ($\Psi \approx \Psi_0$), we get:

$$F \equiv \sum_n \Psi(E_n,r)\Psi^*(E_n,r') + \frac{1}{2\pi}\int_0^{\sqrt{2mE_{max}}} [\Psi(E,r)\Psi^*(E,r') - 4\sin kr \cdot \sin kr']\,dk = 0. \qquad (8)$$

For $r_1 \le r \le a$, $r \neq r'$ the expression F in the left-hand side of eq. (8) is a function of parameter V_1, and is equal to zero if V_1 is the value of the first step of unknown potential. Instead of zero point for F we can look for a required value V_1, from the minimum condition for the expression

$$|F(V_1, r, r')| + |F(V_1, r, r'')| + \ldots; \quad r', r'' \ldots \neq r$$

or

$$\int |F(V_1, r, r')|^2 \, dr'. \qquad (9)$$

So the first step of solving the inverse scattering problem is completed. Proceeding in the same manner and using instead of (5), (6) the continuity conditions of Ψ and Ψ' at other points r_i, the values V_i can be determined also for other intervals of the interaction region.

3. RECONSTRUCTION OF A POTENTIAL FROM R-MATRIX RESONANCES AND THEIR REDUCED WIDTHS

For the potentials of finite range a it is convenient to use the fact, that the solutions of Schroedinger equation (1) with the homogeneous boundary conditions at $r=0$ and $r=a$:

$$U(0)=0; \quad U'(a)/U(a)=B=\text{const} \tag{10}$$

form a discrete set of Hamiltonian eigenfunctions $U_\lambda(r)\equiv U(E_\lambda,r), \lambda=1,2,\ldots$, satisfying the completeness condition in interval $(0,a)$:

$$\sum_\lambda U_\lambda(r)U_\lambda(r')=\delta(r-r'). \tag{11}$$

Due to this fact the scattering data are parametrized by a discrete set of constants E_λ , γ_λ^2. So, for an R-matrix (which uniquely determines an S-matrix) we have:

$$R(E)=\sum_\lambda \frac{\gamma_\lambda^2}{E_\lambda-E}; \quad \gamma_\lambda=\sqrt{\frac{1}{2ma}}U_\lambda(a). \tag{12}$$

The Parseval equality in form (11), simplifies the solution of the inverse problem in the framework of R-matrix theory (reconstruction of $V(r)$ from E_λ , γ_λ^2). The corresponding procedure is similar to that described in the preceding section: it is only necessary to replace the integrals over the energy variable by sums over λ. So, the amplitudes $A_{l\lambda}$, $B_{l\lambda}$ are expressed as functions of V_l for $E_\lambda > V_l$

$$A_{l\lambda}\sin k_{l\lambda}a + B_{l\lambda}\cos k_{l\lambda}a = U_\lambda(a)=\gamma_\lambda\sqrt{2ma} \tag{13}$$

$$k_{1\lambda}[A_{1\lambda}\cos k_{1\lambda}a - B_{1\lambda}\sin k_{1\lambda}a] = U'_{\lambda}(a) = B\gamma_{\lambda}\sqrt{2ma} \qquad (14)$$

instead of (5), (6). The similar equations have to be written for $E_{\lambda}<V_1$ (we must only use exponentially increasing and decreasing solutions instead of oscillating ones $\sin k_{1\lambda} r$, $\cos k_{1\lambda} r$).

The value of parameter V_1, is determined by minimizing the expression

$$F^2 = \| \sum_{\lambda=1}^{\lambda_{max}} (U_{\lambda}(r)U_{\lambda}(r') - \mathring{U}_{\lambda}(r)\mathring{U}_{\lambda}(r'))\|^2 \qquad (15)$$

4. CONTROL CALCULATIONS

The proposed method of approximate solving the inverse scattering problem was verified by numerical reconstruction of a number of potentials of different shapes from the sets of R-matrix parameters E_{λ} , γ_{λ}^2 corresponding to the lowest part of the spectrum.

At first the direct problem was solved: for definite potential V(r) the set $\{E_{\lambda}, \gamma_{\lambda}^2\}$ with $E_{\lambda} \leq E_{max}$ was determined. Than, according to the procedure described in sect.3. the approximate step potential $V_{step}(r) \approx V(r)$ was found.

Since the reconstruction of a potential belongs to uncorrectly determined problems, the algorithm of calculation of the values V_{step} was regularized following Tichonov /7/. So, instead of the minimum of the expression F^2 of type (15) for every step, we can look for the minimum of

$$F^2 + \alpha\| V_i - V_{i-1} \|^2 \qquad (16)$$

Addition of the term $\alpha(V_i - V_{i-1})^2$ reduces too large variations in potential values V_{step} on the neighbouring steps (i.e, stabilizes the solution of the inverse problem). The coefficient α has to be chosen sufficiently small, in order to distort not too strongly the relation which follows from the Parseval equation and which determines the value of V_i.

As an example, the results of calculations for a particular shape of a potential are shown in the figure.

5. DIFFERENT MODIFICATIONS OF THE METHOD

A better approximation may be achieved if the auxiliary potential is not required to be piecewise constant ($V(r) = const$ for $r_i \leq r < r_{i-1}$).

Thus, in particular, the first potential step can be substituted by a tail of some potential decreasing with $r \to \infty$ which depends on a single free parameter (for example, $V(r \geq r_1) = V_1 e^{-\mu_1 r}$, where V_1 or μ_1 or some connection between V_1 and μ_1 is fixed) and for which the Schroedinger equation is solved analytically. Let $f(r)$ and $g(r)$ be such two linearly independent solutions. Then, the wave function Ψ can be represented for $r \geq r_1$ in the form:

$$\Psi(r \geq r_1) = A_1 f(r) + B_1 g(r) \qquad (17)$$

and the coefficients A_1 and B_1 can be expressed through the known scattering matrix and the free potential parameter, which is determined from the completeness condition, as it was shown in the preceding sections.

Simple steps can be substituted by the potentials dependent on several parameters in all the other coordinate intervals $[r_i, r_{i-1}]$ assuming the analytical solvability of the corresponding Schroedinger equations. For example, we can choose $V(r_i \le r \le r_{i-1}) = C_i + V_i e^{-\mu_i r}$ and require that the three parameters C_i, V_i, μ_i are connected by two conditions: the continuity and the smoothness of the sewing at $r = r_{i-1}$ of parts of a potential in the neighbouring intervals. Then the single free potential parameter is fixed by the completeness condition as before.

It is clear that the step approximation does not prevent to take into account exactly the centrifugal barrier $\ell(\ell+1)/r^2$ and the Coulomb forces ze/r, because the addition of potential energy V_i, which is constant in the interval $[r_i, r_{i-1}]$ does not break the analytical solvability of the Schroedinger equation for $r_i \le r \le r_{i-1}$.

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