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A MODEL OF THE INVERSE SCATTERING PROBLEM IN NUCLEAR PHYSICS

(A finite-difference approximation for the Schroedinger equation)

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A MODEL OF THE INVERSE SCATTERING PROBLEM IN NUCLEAR PHYSICS

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1. INTRODUCTION

Recently /1,2/ the inverse problem was formulated in R-matrix scattering theory for finite range potentials and potentials which are not known inside a bounded region. In comparison with the general case the inverse problem is sufficiently simplified in R-matrix theory. As the initial information for reconstruction of interaction the pure discrete set of scattering parameters (R-matrix resonance positions E_λ and their reduced widths γ_λ) is then exploited instead of S-matrix which is a continuous function of energy.

In the finite-difference approximation for the Schroedinger equation an additional simplification of the reconstruction procedure for potential is achieved /3/. The number of spectral points E_λ becomes finite ($\lambda = 1, \ldots N$) like the number of finite-difference intervals into which the region of interaction is divided. The integral equations of the inverse problem are then transformed into a system of the finite number of algebraic equations. So some algebraic analog of the Gelfand-Levitan-Marchenko theory (see, for example /4, 5, 6/) is obtained.

In this paper a method of determining the interaction which does not require solution even of this system of algebraic equations is given. A potential is calculated in a sequence of points by a simple recurrent relation (see (9), (10)). As in /3/ we get here the exact inverse problem in the finite-difference R-matrix theory: from parameters $\{E_\lambda, \gamma_\lambda\}$ which correspond to a definite potential $V(n)$ the same values of $V(n)$ are reconstructed. This fact and the extreme simplicity of the formalism make the method useful as a model for investigation of

some complicated problems of quantum theory. Thus, for example , we may hope to clarify the question about the "complete experiment" for different nuclear systems (determination of relations between scattering parameters).

The class of problems to which the considered here approach corresponds, enlarges due to the generalization of this method to the cases of complex-valued potentials, multichannel systems, nonlocal interactions, equations with partial differences (many dimensions), the systems of many interacting particles.

The numerical calculation algorithm of this method is simple for programming and is suitable for realization by computer: the same formulae (9), (10) are used many times.

By control numerical solution of the direct and corresponding inverse scattering problem for a set of arbitrary chosen potentials $V(n)$, the difference between the initial and resulting values of potentials was about $10^{-4}\%$ (for $N \approx 10\text{-}20$)*.

2. *DIRECT PROBLEM*

Before we shall describe the new reconstruction procedure of interaction from scattering data $\{E_\lambda, \gamma_\lambda\}$ we shall remind some points concerning the solution of the finite-difference Schroedinger eq.($h = m = 1$):

$$-\frac{1}{2}[u_\lambda(n+1)-2u_\lambda(n)+u_\lambda(n-1)]/\Delta^2+V(n)u_\lambda(n)=E_\lambda u_\lambda(n), \qquad (1)$$

where Δ is a finite-difference coordinate step. The potential $V(n)$ is assumed to be of finite range "a" ($V(n \geq N=a/\Delta)=0$) or it is known for $n \geq N = a/\Delta$.

Homogeneous boundary conditions, which are used for basic functions in the R-matrix scattering theory, are:

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*The calculation of several variants required about 20 seconds (computer BESM-6).

$$u_\lambda(0)=0; \quad u_\lambda(N+1) = u_\lambda(N)(1+\Delta B/a). \qquad (2)$$

Equations (1)-(2) give a system of N homogeneous algebraic equations for N unknown values of eigenfunctions $u_\lambda(1), u_\lambda(2)\ldots u_\lambda(N)$ on the interval $0<n\leq N$.

This system has solutions at N energy eigenvalues $E=E_\lambda$.

The eigenfunctions $u_\lambda(n)$ are orthogonal to each other for $E_\lambda \neq E_{\lambda'}$ and can be normalized according to the orthonormality relation:

$$\sum_{n=1}^{N} \Delta \cdot u_\lambda(n)\, u_{\lambda'}(n) = \delta_{\lambda\lambda'}. \qquad (3)$$

They compose a complete set of functions determined at N points of interval $0<n\leq N$ and obey the completeness relation (orthogonality with respect to the energy variable E_λ):

$$\sum_{\lambda=1}^{N} u_\lambda(n)\, u_\lambda(m) = \delta_{mn}/\Delta. \qquad (4)$$

The parameters E_λ and $u_\lambda(N) \equiv \gamma_\lambda \sqrt{2a}$ determine the R-matrix

$$R(E) = \sum_{\lambda}^{N} \frac{\gamma_\lambda^2}{E_\lambda - E} \qquad (5)$$

which is connected with the scattering matrix $S(E)$ /3,7/.

3. *INVERSE SCATTERING PROBLEM*

The inverse problem in R-matrix scattering theory is as follows: we have to find a potential $V(n)$, $0<n<N$ using as an input information the set of parameters $\{E_\lambda, \gamma_\lambda\}$.

Thus, we know E_λ , $u_\lambda(N) \equiv \gamma_\lambda \sqrt{2a}$ and $u_\lambda(N+1)$ connected with $u_\lambda(N)$ according to (2), and the value $V(N)$ (which is equal to zero, if the potential range is $<a = N\cdot\Delta$).

Fixing in the Schroedinger equation (1) $n = N$ we get the values of eigenfunctions in the first internal point, where the interaction is not known:

$$u_\lambda(N-1) = 2\Delta^2[\,V(N) - E_\lambda + 1/\Delta^2\,]\,u_\lambda(N) - u_\lambda(N+1). \qquad (6)$$

Writing now eq. (1) for $n = N-1$

$$-\frac{1}{2}[u_\lambda(N) - 2u_\lambda(N-1) + u_\lambda(N-2)]/\Delta^2 + V(N-1)u_\lambda(N-1) = E_\lambda u_\lambda(N-1), \qquad (7)$$

we get one equation for two unknown values $u_\lambda(N-2)$ and $V(N-1)$ which is not sufficient to determine them. But, if we multiply both the sides of eq. (7) by $u_\lambda(N-1)\cdot\Delta$ and summarize them over λ, using the orthogonality condition (4), we get:

$$V(N-1) = \Lambda \sum_{\lambda=1}^{N} E_\lambda u_\lambda^2(N-1) - \frac{1}{\Delta^2}. \qquad (8)$$

So, according to eqs. (6) and (8) $u_\lambda(n)$ and $V(n)$ at the point $n = N-1$ are determined (one step inside the region, where we look for the values of interaction). Repeating the same procedure in subsequent points, using recurrent relations

$$u_\lambda(n) = 2\Delta^2[\,V(n+1) - E_\lambda + \frac{1}{\Delta^2}\,]\,u_\lambda(n+1) - u_\lambda(n+2); \qquad (9)$$

$$V(n) = \Delta \sum_{\lambda=1}^{N} E_\lambda u_\lambda^2(n) - \frac{1}{\Delta^2}, \qquad (10)$$

we get the solution of the inverse scattering problem. The results of control numerical calculations (for $N = 10$) are given in the table. For several arbitrary chosen potentials $V(n)$ the sets $\{E_\lambda, \gamma_\lambda\}$ were determined (solution of direct problem), and used as initial data for inverse problem. The reconstructed potentials $\tilde{V}(n)$ have appeared to be very close to $V(n)$. The calculations with double number of steps ($N = 20$) in the interval $0 < n\cdot\Delta \le a$ have given also a very good accordance of $V(n)$ and $\tilde{V}(n)$.

The number of operations which are required for finding the potential in this method is proportional to N^2.

Table

Comparison of initial potential values V(n) with those derived by solving the direct and the corresponding inverse problem. 1 - pure repulsion, 2 - attraction + repulsion; 3 - pure attraction.

n	Variant 1		Variant 2		Variant 3	
	V(n)	$\tilde{V}(n)$	V(n)	$\tilde{V}(n)$	V(n)	$\tilde{V}(n)$
1	65.1000	65.0998	-10.0000	-10.0000	- 10.0000	-10.0001
2	53.2000	53.2001	-10.0000	-10.0000	- 10.0000	-10.0013
3	32.5000	32.5001	-10.0000	-10.0000	- 10.0000	-9 .99914
4	30.2000	30.2000	-10.0000	-10.0000	- 10.0000	- 9.99973
5	28.4000	28.4000	-10.0000	-10.0000	- 10.0000	- 9.9999
6	25.6000	25.6000	-10.0000	-10.0000	- 10.0000	-10.0011
7	21.8000	21.8000	+10.0000	+10.0000	- 10.0000	- 9.99921
8	16.0000	16.0000	+10.0000	+10.0000	- 10.0000	- 9.99994
9	9.4000	9.4000	+10.0000	+10.0000	- 10.0000	- 9.99992
10	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

It is much easier in comparison with the finite-difference (algebraic) analog of Gelfand-Levitan procedure in R-matrix scattering theory /3/ *, where this number is proportional to N^4.

The proposed method can be modified in order to reconstruct potentials directly from scattering phase shifts, instead of R-matrix parameters E_λ, γ_λ using a complete set of eigenfunctions dependent on the coordinate variable in the infinite interval $0<n<\infty$ and not only in the region $0<n\leq N$ where we look for $V(n)$. In the case of continuous coordinate such a complete set is formed of solution with the asymptotic behaviour

$$\Psi_E(x) \to \sqrt{\frac{2}{\pi}} \sin(k x + \delta(E)) , \qquad (11)$$

where $\delta(E)$ is the scattering phase shift. The completeness relation in this case is (if there are no bound states):

$$\int_0^\infty \Psi_E(x)\,\Psi_E(x')\,dE = \delta(x-x') . \qquad (12)$$

For the finite-difference analog $\Psi_E^{f-d}(n)$ of the solution $\Psi_E(x)$ (continuous spectrum of solutions $\Psi_E^{f-d}(n)$ of eq. (1) has an upper bound $E_{max} \sim \frac{1}{\Delta^2}$) we get:

$$\int_0^{E_{max}} \Psi_E^{f-d}(n)\,\Psi_E^{f-d}(m)\,dE = \delta_{mn}/\Delta \qquad (13)$$

instead of (12).

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* In paper /3/ the following corrections are to be done:

$$\Phi(E,N)=\sqrt{2a}\,;\quad \gamma_\lambda \equiv u_\lambda(N)/\sqrt{2a}\,;\quad K(n,n)=1\,;\quad q(m,n)+$$

$$+\sum_{p=m+1}^{N} K(m,p)q(p,n)=0 \ \text{ for } m<n\,;\quad V(n)=\frac{1}{2\Delta^2}[K(n+1,n)-$$

$$-K(n,n-1)]\,;\quad \Psi(E,N)=I(E,N)-S(E)O(E,N)$$

and corresponding corrections in the matrix analog to these relations.

The orthonormalization relation (13) can be used for reconstruction of potentials, which are not known at $n < N$*.

Recurrent relations (9), (10) are then replaced by

$$\Psi_E^{f-d}(n) = 2\Delta^2\left[V(n+1) - E + \frac{1}{\Delta^2}\right]\Psi_E^{f-d}(n+1) - \Psi_E^{f-d}(n+2) \qquad (14)$$

$$V(n) = \Delta \int_0^{E_{max}} E\,[\Psi_E^{f-d}(n)]^2\,dE - \frac{1}{\Delta^2} . \qquad (15)$$

APPENDIX

Some Possible Ways of Generalization of the Formalism

I. Writing (1)-(10) in the matrix form, the inverse problem can be solved for multichannel processes in nuclear systems. A generalization of the finite-difference R-matrix formalism to the case of coupled-channels is made in /2,3/ **. Here we give, for brevity, only recurrent relations of type (9), (10) for α-components of eigenfunctions and elements of interaction matrix

$$u_{\alpha\lambda}(n) = 2\Delta^2 \sum_{\alpha'} V_{\alpha\alpha'}(n+1)\,u_{\alpha'\lambda}(n+1) + 2u_{\alpha\lambda}(n+1)(1-\Delta^2 E_\lambda) -$$

$$-u_{\alpha\lambda}(n+2)\,; \qquad (16)$$

$$V_{\alpha\alpha'}(n) = \Delta \sum_{\lambda=1}^{N} E_\lambda u_{\alpha\lambda}(n)\,u_{\alpha'\lambda}(n) - \frac{\delta_{\alpha\alpha'}}{\Lambda^2} . \qquad (17)$$

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* The inverse problem can be solved using the functions ϕ and $\overset{0}{\phi}$ and the orthogonality of $\phi(E,m)$ and $\overset{0}{\phi}(E,n)$ (if $m<n$) as functions dependent on E.

** The problem of connection of partial reduced widths $\gamma_{\alpha\lambda}$ corresponding to closed channels with scattering matrix elements remains here unsolved as in refs /2,3/.

2. The case of complex value interaction distinguishes (in comparison with real potential cases) only in replacing the orthogonality property of functions u_λ by *biorthogonality* of sets of conjugate eigensolutions $\{u_\lambda\}, \{u^*_\lambda\}$

$$\sum_\lambda (u^*_\lambda(n))^* u_\lambda(m) = \sum_\lambda u_\lambda(n) u_\lambda(m) = \delta_{mn}/\Delta$$

instead of

$$\sum_\lambda u^*_\lambda(n) u_\lambda(m) = \delta_{mn}/\Delta .$$

3. As an example of the multidimensional inverse problem it is appropriate to consider the two dimensional case: reconstruction of a potential $V(n,m)$ in the region Ω from the values E_λ and $\gamma_{\lambda s} \sim u_\lambda(s)$ where s denotes a point on the boundary of Ω. Instead of the Schroedinger equation in ordinary finite differences (1) we have here the equation in partial differences/5,8/ which connects the values of solutions in five neighbouring points on the plane:

$$-\frac{1}{2\Delta^2}[u_\lambda(n,m+1) + u_\lambda(n+1,m) + u_\lambda(n,m-1) + u_\lambda(n-1,m) -$$

$$- 4u_\lambda(n,m)] + V(n,m)\, u_\lambda(n,m) =$$

$$= E_\lambda u_\lambda(n,m) . \qquad (18)$$

Eigenfunctions u_λ which satisfy the homogeneous boundary conditions (e.g., the constancy of the partial difference derivative on S) form a complete set in Ω. The corresponding energy eigenvalues E_λ and $u_\lambda(s)$ (scattering parameters) determine the R-matrix

$$R_{ss'}(E) = \sum_\lambda \frac{\gamma_{\lambda s}\, \gamma_{\lambda s'}}{E_\lambda - E} . \qquad (19)$$

As an analog of (9), (10) there are the formulae which express $u_\lambda(m,n)$ and $V(m,n)$ at a point (m,n) inside the region of unknown interaction through the values E_λ and u_λ (in four neighbouring points), which are determined at the preceding stage of solution of the problem.

The utilization of such recurrent relations of the finite-difference inverse problem permits one to get explicitly the mutual dependence of different scattering data in multidimensional case. Thus we have here a possibility to understand one of the very difficult questions in quantum theory. For instance, it is easy to see that for the rectangular region it is enough to know the values $\gamma_{\lambda s}$ on one of its sides ($s \in S^I$) in order to determine u_λ in the whole Ω including the remaining part of the boundary ($\gamma_{\lambda s'} \notin S^I$) by moving over the finite-difference net and taking into account the boundary conditions for u_λ*.

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*The connection of scattering parameters can be useful for phase analyses, because it gives additional relations to determine from cross sections not only the moduli of scattering amplitudes but also their phases.