Inverse scattering problem (finite-difference approach)

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It is shown that the main logical points of the inverse scattering problem become especially clear in the framework of R-matrix scattering theory in the finite-difference approximation for the Schrödinger equation. Within a unified scheme, different methods are presented for determining the interaction from scattering data in single-channel, many-channel, and many-particle systems, for which exactly solvable finite-dimensional models of the inverse problem are constructed.

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INTRODUCTION

For more than half a century physicists have been solving the *direct problem*: $V \to S$; that is, from a given interaction V, use the Schrödinger equation to find the wave function Ψ of a definite investigated object and from this function determine all its properties (symbolically denoted by S, which, in particular, can be the scattering matrix). But the forces acting in the investigated system are not known in advance and one needs to recover V from experimentally determined S.[1)] This is the *inverse problem*: $S \to V$.

It was only 25 years after the discovery of the Schrödinger equation that Gel'fand, Levitan, and Marchenko[1,2] laid the foundations of the theory of the inverse problem. And although important successes have been achieved in the meanwhile,[3] potentials are still found by the direct method (by trial and error).

One can identify a number of reasons for this. The mathematical formalism of the inverse problem is rather complicated. For the unique determination of V in the classical formulation, it is necessary to know the phase shifts at energies $E \to \infty$. The stability of the procedure $S \to V$ is not sufficiently clear. All this creates a certain psychological barrier which discourages many physicists from mastering the fundamentals of the theory.

It has however been shown recently[2)] that combination of R-matrix scattering theory with ordinary scattering theory and solution of the differential equations on a computer by the finite-difference approximation significantly facilitate the exposition and understanding of the inverse problem methods. Furthermore, a method has since been found for determining the interaction from the scattering data (also in the finite-difference approximation for the equations of motion) which is of comparable simplicity with the solution of the direct problem.

In the present review, these results are used, first, to illustrate the main points of the inverse problem (above all, the fundamental role of the completeness property of the system of eigenfunctions). Then, in a unified scheme, the main methods of the inverse problem are presented. In this way, the ideas of the theory are readily comprehended, and this may be helpful to anyone studying quantum phenomena.

It is remarkable that in finite-difference R-matrix theory, the finding of V requires only a *finite* number of scattering parameters (positions of resonances E_λ and their reduced widths γ_λ) determined from experimental data over a bounded energy range. This automatically removes the difficulty of allowing for states with $E \to \infty$. Moreover, when the inverse problem is formulated in this way, an *exact* connection is established between the scattering data and the interaction and it is necessary to perform only a *finite* number of *purely algebraic* operations to determine V from E_λ and γ_λ. The method is therefore very convenient when used as a model to investigate a number of complicated questions of quantum theory. This applies particularly to the question of the minimum amount of information needed to determine V, i.e., the problem of the complete experiment and the connections between different scattering data.

In the review, we consider one-dimensional motion of particles in an external field and we generalize the inverse problem to systems with strong coupling of channels. The new approach used in the review then makes it possible to go over without difficulty to even the multidimensional case, for which the inverse problem long defied solution.[3] Examples of the determination of the interaction of three (and more) particles are discussed.

This review cannot replace other reviews,[3,8–13] but can only complement them with a new understanding of the inverse problem theory. Some of the results obtained by the authors are published here for the first time.

1. ELEMENTARY EXAMPLE OF A SOLUTION OF THE INVERSE PROBLEM

The main difficulty encountered by physicists when they begin to study the inverse problem is something which gets lost in the traditional approaches: the logical connection between the many stages in the construc-

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[1)] It is assumed that a phase-shift analysis of the experimental data has been performed and we know the S matrix or equivalent quantities (phase shifts, R matrix, etc). The problems related to this analysis will not be considered here.

[2)] The finite-difference analog of Gel'fand–Levitan–Marchenko inverse problem methods was proposed by Case and Kac[4,5] and for R-matrix finite-difference theory by Zakhar'ev *et al.*[6]

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tion of V from the scattering data S. He who does not know the spectral theory of operators may not understand, why, for example, in the Gel'fand–Levitan approach, one first constructs the so-called *spectral function* ρ from the scattering data. Why, to calculate V from ρ and special auxiliary functions $\mathring{\varphi}$, must one first find a function of two variables, which serves merely as the kernel of an integral equation for a new intermediate function K, which is finally related to the required V (see Sec. 3)?

The traditional approaches will be discussed in the following sections; here we only consider an elementary example of the inverse problem, which is especially convenient for making acquaintance with the theory. For example, one can immediately see why completeness of the set of solutions of the Schrödinger equation is an important additional relation for finding V.

We shall illustrate two variants of solution of the finite-difference inverse problem that use different types of completeness relation (for wave functions Ψ defined on the half axis $(0, \infty)$ and for auxiliary functions u_λ defined in the interval $[0, a]$, the finite range of the interaction).

Finding V and Ψ from the asymptotic behavior of Ψ

We write the one-dimensional Schrödinger equation for the wave function Ψ defined by the conditions

$$\Psi(E, 0)=0;\ \Psi(E, r) \xrightarrow[r\to\infty] (1/k)[\exp(-ikr)-S\exp(ikr)].$$

in the form

$$-\tfrac{1}{2}\Psi''(E, r)+V(r)\Psi(E, r)=E\Psi(E, r). \quad (\hbar=m=1) \tag{1}$$

The finite-difference analog of (1) is the equation

$$-\frac{1}{2\Delta^2}[\Psi(E, n+1)-2\Psi(E, n)+\Psi(E, n-1)] + V(n)\Psi(E, n)=E\Psi(E, n), \tag{2}$$

where the first term on the left is the second finite-difference derivative of $\Psi(E, n)$; $\Delta \equiv r_{n+1}-r_n$ is the step in the finite-difference differentiation; $\Psi(E, r_n)\equiv\Psi(E, n)$; $V(r_n)\equiv V(n)$.

Suppose the required potential has a finite range a: $V(r_n \geq a = N\Delta)\equiv V(n\geq N)=0$. Suppose first that there are no bound states in the field $V(n)$. Outside the range of the potential, the wave function is a combination of the free incident wave I and the scattered wave O [which go over in the limit $\Delta\to 0$ into $\exp(\pm i kr)$; see (45)–(48)]:

$$\Psi(E, n\geq N)=A[I(E, n)-S(E)O(E, n)];\ (\Psi(E, 0)=0), \tag{3}$$

where $S(E)$ is the S matrix; $A^2=(2E-E^2\Delta^2)^{-1/2}\to_{\Delta\to 0} 1/k$ In the inverse problem one must find $V(n)$ given $S(E)$, or, equivalently, from the asymptotic behavior of $\Psi(E, n\geq N)$ since $I(E, n)$ and $O(E, n)$ in (3) are known solutions. But the asymptotic behavior of Ψ is uniquely determined by the values of the wave function $\Psi(E, N)$ and its finite-difference derivative $[\Psi(E, N+1)-\Psi(E, N)]/\Delta$ on the boundary of the interaction region. Therefore, the inverse problem can also be formulated as follows:

Find $V(n)$ from given $\Psi(E, N)$ and $\Psi(E, N+1)$.

Recursion Relations. For each fixed n, Eq. (2) relates the wave function at three neighboring points $(n,\ n\pm 1)$. For $n=N$, $\Psi(E, N-1)$ can be expressed by means of (2) in terms of known $\Psi(E, N)$ and $\Psi(E, N+1)$ by using $V(N)=0$:

$$\Psi(E, N-1)=2\Delta^2[V(N)-E+1/\Delta^2]\Psi(E, N)-\Psi(E, N+1). \tag{4}$$

Thus, Ψ is found at a point where V is unknown. In Eq. (2), now set $n=N-1$:

$$(-1/2\Delta^2)[\Psi(E, N-2)-2\Psi(E, N-1)+\Psi(E, N)] + V(N-1)\Psi(E, N-1)=E\Psi(E, N-1). \tag{5}$$

This is one equation for the two unknowns $\Psi(E, N-2)$ and $V(N-1)$. To eliminate the superfluous unknown, we use the orthogonality relation for the wave functions, not one with respect to the spatial variable n:

$$\frac{1}{2\pi}\sum_n \Delta\Psi^*(E, n)\Psi(E', n)=\delta(E-E'), \tag{6}$$

but one with respect to the energy:

$$\frac{1}{2\pi}\int \Psi(E, m)\Psi^*(E, n)\,dE=\delta_{mn}/\Delta, \tag{7}$$

which is usually called the *completeness condition*[3] (or Parseval's equation; δ_{mn}/Δ is the finite-difference analog of the δ function). Multiply both sides of Eq. (5) by $\Psi^*(E, N-1)$, calculated earlier, and integrate with respect to the energy. This eliminates the unknown $\Psi(E, N-2)$ because $\Psi(E, N-1)$ and $\Psi(E, N-2)$ are orthogonal. The result is an expression for $V(N-1)$ in terms of known quantities:

$$V(N-1)=(\Delta/2\pi)\int E|\Psi(E, N-1)|^2\,dE-1/\Delta^2. \tag{8}$$

Thus, from $\Psi(E, N)$ and $\Psi(E, N+1)$ we have determined $\Psi(E, N-1)$ and $V(N-1)$, i.e., we have advanced one step into the required interaction region and completed the first step in the solution of the inverse problem.

Repeating the procedure at subsequent points, we obtain the *recursion* relations

$$\Psi(E, n)=2\Delta^2[V(n+1)-E+1/\Delta^2]\Psi(E, n+1)-\Psi(E, n+2); \tag{9}$$

$$V(n)=(\Delta/2\pi)\int E|\Psi(E, n)|^2\,dE-1/\Delta^2. \tag{10}$$

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[3] For it follows from (7) that any function $f(m)$ can be expanded with respect to the set of wave functions $\Psi(E, m)$. Multiplying both sides of (7) by $f(n)$ and summing over n, we obtain.

$$f(m)=\int C(E)\Psi(E, m)\,dE,$$

where

$$C(E)=\sum_n \Delta\Psi^*(E, n)f(n).$$

Using them, we find the wave function and potential in the complete region $n<N$ from known $\Psi(E,N)$, $\Psi(E,N+1)$. Thus, the procedure for solving the inverse problem posed above is not greatly more complicated than in the case of the direct problem.

Energy Cutoff. In the derivation of the recursion relations (9) and (10), we have not drawn attention to the important circumstance that the spectrum of states Ψ, which is a complete set, is bounded above in the finite-difference approximation for the Schrödinger equation. The integration with respect to E in (7), (8), and (10) is from 0 to $E_{max}=2/\Delta^2$. This rigorous mathematical fact can be illustrated by the simple example of free motion. The complete set of solutions of (1) with $V=0$ consists of real oscillating functions with all possible frequencies from zero to infinity [they are linearly independent and orthogonal in accordance with (6)]. But in the finite-difference case, there is no frequency at all greater than the maximal $k=2/\Delta$. This greatest frequency corresponds to $E=E_{max}=2/\Delta^2$. Hence, the complete set of states with all frequencies permitted by Eq. (2) is exhausted for $E\leqslant E_{max}=2/\Delta^2$.

Bound States. So far we have assumed the absence of bound states in the system. But if the potential $V(n)$ has M discrete levels with $E=E_i(i=1, 2, \ldots, M)$, then the integrals with respect to the energy in (7)–(10) must be augmented by sums over the bound states. Their functions $\Psi(E_i, n)$ are normalized to unity:

$$\sum_{n=1}^{N}\Delta\Psi^2(E_i, n)=1. \tag{11}$$

To solve the inverse problem in this case, we need to known not only $\Psi(E, N)$, $\Psi(E, N+1)$ $(0\leqslant E\leqslant E_{max})$ but also $\Psi(E_i, N)$, $\Psi(E_i, N+1)$ $(i=1, 2, \ldots, M)$. The asymptotic behavior of $\Psi(E_i, n\geqslant N)$ is the free solution of (2) with $V=0$ which decreases with n and has amplitude A_i. Thus, specification of $\Psi(E_i, N)$ and $\Psi(E_i, N+1)$ is equivalent to specifying the energies E_i of the bound states and the corresponding constants A_i, which can be found experimentally.[14]

Potentials with known "Tail." It was assumed above that $V(n\geqslant N)=0$. But the procedure proposed for solving the inverse problem can also be extended to the case when V for $n\geqslant N$ has nonzero but known values $V(n)\to 0$ as $n\to\infty$. Since the wave functions are known for $n\geqslant N$, one can find from E_i and given $S(E)$ and A_i the values of Ψ at the points N and $N+1$, which are used as input information in the inverse problem described above.

Inverse problem in finite-difference R-matrix theory (completeness on $(0,a]$)

The procedure for solving the inverse problem takes on its simplest form in the finite-difference formalism of R-matrix scattering theory. Although we did assume above that the required potential has a finite range, this *a priori* information was not fully used. In fact, if it is used, the number of input data required to determine $V(n)$ can be greatly reduced.

If we rely on completeness of the set of solutions (2), not on the complete half-axis $(0, \infty)$, but only on the interval $(0, a]$, where the potential is sought, the continuous spectrum is replaced by the discrete spectrum of eigenstates of the Hamiltonian at a finite number of energies $E=E_i(i=1, \ldots, N)$. For this, we choose the auxiliary solutions $u(E, n)$ of Eq. (2) used in R-matrix scattering theory as basis functions (the finite-difference variant of this theory is set forth in Appendix 1). The functions $u(E, n)$ are specified by homogeneous boundary conditions at the ends of the interval $[0, a]$:

$$u(E, 0)=0;\ u(E, N-1)=u(E, N)(1+\Delta B/a). \tag{12}$$

The second condition in (12) corresponds to equality of the certain constant B/a to the finite-difference logarithmic derivative $[u(E, n+1)-u(E, n)]/\Delta u(E, n)$ at the point $n=N$.[4)]

It is well known that such a system has solutions only at N values of the energy $E=E_\lambda(\lambda=1, 2, \ldots, N)$. The relations of orthogonality and completeness for $u_\lambda(n)\equiv u(E_\lambda, n)$ are the discrete (with respect to the energy) analogs of (6) and (7) and are (derivation in Appendix 2)

$$\sum_{n=1}^{N}\Delta u_\lambda(n)u_{\lambda'}(n)=\delta_{\lambda\lambda'}; \tag{13}$$

$$\sum_{\lambda=1}^{N}u_\lambda(n)u_\lambda(m)=\delta_{mn}/\Delta; \tag{14}$$

R-matrix scattering theory makes it possible to parametrize the continuous energy dependence of the S matrix by means of the discrete E_λ (the positions of the resonances) and the values of the eigenfunctions u_λ at the boundary of the interaction region (reduced widths of the resonances). In the finite-difference approximation, there are altogether $2N$ of these parameters: $\{E_\lambda, \gamma_\lambda\}$. The R matrix, which is uniquely related to $S(E)$ (see Appendix 1), has the simple form

$$R(E)=\sum_{\lambda}^{N}[\gamma_\lambda^2/(E_\lambda-E)]. \tag{15}$$

Thus, we obtain a new formulation of the inverse problem:

Find $V(n)$ from given E_λ, $\gamma_\lambda(\lambda=1, \ldots N)$.

Recursion Relations. In the formulation given above, the solution of the inverse problem can be reduced to the use of recursion relations, which differ from (9) and (10) only by the replacement of integrals by finite sums:

$$u_\lambda(n)=2\Delta^2[V(n+1)-E_\lambda+1/\Delta^2]u_\lambda(n+1)-u_\lambda(n+2); \tag{16}$$

$$V(n)=\Delta\sum_{\lambda=1}^{N}E_\lambda u_\lambda^2(n)-1/\Delta^2. \tag{17}$$

In this case, to determine $V(n)$ for $n<N$ one needs to perform purely algebraic operations, and a strictly finite number of them! Equations (16) and (17) establish an exact and unique correspondence between the

[4)] The conditions (12) make it possible to eliminate $u(E, 0)$ and $u(E, N+1)$ from Eq. (2) for $u(E, n)$ and separate a closed system of N homogeneous algebraic equations for $u(E, 1)$, $u(E, 2)$, $\ldots$, $u(E, N)$.

scattering parameters $\{E_\lambda, \gamma_\lambda\}$ and the values of $V(n)$.

In contrast to the direct problem, in which the solution of the Schrödinger equation can be obtained at one definite energy, to calculate V in the inverse problem it is necessary to find $u(E, n)$ simultaneously for all values of E corresponding to the complete set of eigenfunctions.

Control Calculations. The algorithm for solving the inverse problem using (16) and (17) is very convenient for realization on a computer (a small number of operations is repeated many times). To test the method for various potentials $V(n)$ of different form (attractive, repulsive, and of variable sign) we first calculated the parameters $\{E_\lambda, \gamma_\lambda\}$. This direct problem here plays the role of a scattering experiment. Then the $\{E_\lambda, \gamma_\lambda\}$ values were used as input data for the inverse problem. When recovered, the potentials $\tilde{V}(n)$ coincided with $V(n)$ to eight significant figures, which confirmed the exact correspondence $\{E_\lambda, \gamma_\lambda\} \leftrightarrow V(n)$. The slight difference between V and $\tilde{V}$ is explained by the given finite accuracy limit of computer calculations (in the 10th place). The calculation is rather stable against "machine errors" (for $N = 20$ after the cycle through the direct and inverse problem the error increased by not more than two orders).

Constraints on the Scattering Parameters. The class of scattering data $\{E_\lambda, \gamma_\lambda\}$ corresponding to a finite-difference Schrödinger equation and finite-range potentials is very restricted. (The number of independent scattering parameters must be equal to the number of points at which $V \neq 0$). They must satisfy N nonlinear equations [in accordance with (12)]:

$$u_\lambda(0) = 0, \tag{18}$$

where the $u_\lambda(0)$ must be replaced by the expressions for them in terms of E_λ and γ_λ obtained by means of Eqs. (16) and (17).

It may be convenient to use $N(N-1)/2$ different constraints, even though these follow from (18). They are obtained from the Schrödinger equation for $u_\lambda(n)$ by multiplying by $u_\lambda(n+m)$ and summing over λ with allowance for (14):

$$\left.\begin{aligned} -1/2\Delta^3 &= \sum_\lambda E_\lambda u_\lambda(n)\, u_\lambda(n-1) \quad \text{for } n = 1, 2, \ldots, (N-1); \\ 0 &= \sum_\lambda E_\lambda u_\lambda(n)\, u_\lambda(n') \quad \text{for } n' > n+1. \end{aligned}\right\} \tag{19}$$

More interesting relations (solvable for γ) between the scattering data are obtained in multidimensional problems (see Sec. 5).

2. ALGEBRAIC ANALOG OF THE GEL'FAND-LEVITAN-MARCHENKO THEORY

The Gel'fand–Levitan–Marchenko inverse problem methods arose as a continuum generalization of the corresponding results of the theory of Jacobi matrices. It would seem that this algebraic theory could not be used directly for scattering problems: It uses purely discrete quantities, whereas particle collisions are described by continuous wave functions corresponding to continuum states of the interaction Hamiltonian of physical systems.

However, as we have already noted above, in the case of finite-range forces the scattering data can be parameterized by a discrete set of constants—the positions E_λ of the resonances and their reduced widths γ_λ (in the framework of R-matrix theory). In conjunction with the finite-difference approximation for the Schrödinger equation, which goes over into a system of algebraic equations with Jacobi matrix for the coefficients, one can obtain a purely algebraic analog of the Gel'fand-Levitan–Marchenko theory that has physical meaning.

Inverse problem in R-matrix theory (finite-difference approximation, method of orthogonalization of polynomials)

Depending on the choice of the boundary conditions, different solutions are obtained to the same Schrödinger equation with the same original potential V. Above, to construct V, we have already used two types of solutions (2): the wave functions Ψ, which are convenient in that the S matrix enters explicitly into the values of Ψ on the boundary of the interaction region (3), and the eigenfunctions $u_\lambda(n)$ corresponding to the conditions (12), whose advantage resides in the finiteness of the number of solutions $u_\lambda(n)$ forming the complete set.

We consider now new types of solution $\varphi(E, n)$ that have a remarkable energy dependence which enables one to relate $\varphi(E, n)$ simply to the known free solutions $\mathring{\varphi}(E, n)$ of Eq. (2) with $V(n) \equiv 0$:

$$(-1/2\Delta^2)[\mathring{\varphi}(E, n+1) - 2\mathring{\varphi}(E, n) + \mathring{\varphi}(E, n-1)] = E\mathring{\varphi}(E, n). \tag{20}$$

Having determined $\varphi(E, n)$, one can readily find $V(n)$ as well from (2).

Auxiliary Solutions. For φ and $\mathring{\varphi}$ inhomogeneous boundary conditions are chosen at the point $r = a$:

$$\left.\begin{aligned} &\varphi(E, N) = \mathring{\varphi}(E, N) = 1/\sqrt{2a};\ \varphi(E, N-1) \\ &\quad = \varphi(E, N)(1 + \Delta B\, a);\ \mathring{\varphi}(E, N-1) = \mathring{\varphi}(E, N)(1 + \Delta B\, a), \end{aligned}\right\} \tag{21}$$

to ensure existence of the solutions φ and $\mathring{\varphi}$ for all E, i.e., to ensure they have a continuous energy dependence.

One of the boundary conditions for φ is specially chosen in the same way as for the eigenfunctions $u_\lambda(n)$ (12) to make the $\varphi(E, n)$ differ from $u_\lambda(n)$ at $E = E_\lambda$, where u_λ are defined, by only a constant factor $\gamma_\lambda \equiv u_\lambda(N)/\sqrt{2a}$:

$$u_\lambda(n) = \gamma_\lambda \varphi(E_\lambda, n). \tag{22}$$

Then the completeness relation of the eigenfunctions u_λ can also be used for φ [substitute (22) into (14)]:

$$\sum_\lambda \gamma_\lambda^2 \varphi(E_\lambda, n)\, \varphi(E_\lambda, m) = \delta_{mn}/\Delta, \tag{23}$$

i.e., like u_λ, the $\varphi(E_\lambda, n)$ are orthogonal with respect to

the energy variable[5] only with the different *weight* γ_λ^2.

Because of the special coupling of the values of the solutions in the finite-difference Schrödinger equation (2), we can now show that each step forward into the interaction region increases by unity the degree of the polynomial dependence of φ on E (at the point N, $\varphi(E, N) = \text{const}$ in accordance with (21), i.e., it is a polynomial of zeroth degree in E). This can be clearly demonstrated by rewriting (2) for φ in matrix form and taking into account (21):

$$\begin{pmatrix} \left[\frac{1-\Delta B\, a}{2\Delta^2}-V(N)\right] & -\frac{1}{2\Delta^2} & 0 & 0 & 0 \\ -\frac{1}{2\Delta^2} & \left[\frac{1}{\Delta^2}-V(N-1)\right] & -\frac{1}{1\Delta^2} & 0 & 0 \\ 0 & -\frac{1}{2\Delta^2} & \left[\frac{1}{\Delta^2}-V(N-2)\right] & -\frac{1}{2\Delta^2} & 0 \\ 0 & 0 & -\frac{1}{2\Delta^2} & \left[\frac{1}{\Delta^2}-V(N-3)\right] & -\frac{1}{2\Delta^2} \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \times \begin{pmatrix} \varphi(N) \\ \varphi(N-1) \\ \varphi(N-2) \\ \varphi(N-3) \\ \vdots \end{pmatrix} = E \begin{pmatrix} \varphi(N) \\ \varphi(N-1) \\ \varphi(N-2) \\ \varphi(N-3) \\ \vdots \end{pmatrix} \tag{26}$$

It is important that the coefficient matrix H of the system of algebraic equations (26) is *tridiagonal.*[6] Because of this, the first equation in (26) relates $\varphi(E, N-1)$ solely to the known constant $\varphi(E, N) = \sqrt{2a}$. Obtaining from this equation an expression for $\varphi(E, N-1)$, we find that the energy enters it only in the form of a factor multiplying $\varphi(E, N) \equiv \sqrt{2a}$. Therefore, $\varphi(E, N-1)$ is a polynomial of first degree in E. Because H is tridiagonal, in each subsequent equation there appears one new unknown function $\varphi(E, N-2)$, $\varphi(E, N-3), \ldots$, and the factor E on the right-hand side of (26) increases by unity the degree of their polynomial dependence on the energy. Thus, $\varphi(E, n)$ is a polynomial of degree $N-n$. This is true of any potential $V(n)$, i.e., for the free solutions $\mathring{\varphi}$ as well.

Construction of φ from $\mathring{\varphi}$. The polynomial $\varphi(E, n)$ of degree $N-n$ can be constructed as a linear combination of polynomials $\mathring{\varphi}(E, m)$ whose degrees decrease from $N-n$ to 0, i.e., $n \leq m \leq N$[7]:

$$\left.\begin{aligned} \varphi(E, N) &= \Delta K(N, N)\,\mathring{\varphi}(E, N); \\ \varphi(E, N-1) &= \Delta K(N-1, N-1)\,\mathring{\varphi}(E, N-1) \\ &\quad + \Delta K(N-1, N)\,\mathring{\varphi}(E, N); \\ &\cdots\cdots\cdots\cdots\cdots\cdots \\ \varphi(E, n) &= \Delta K(n, n)\,\mathring{\varphi}(E, n) + \ldots + \Delta K(n, N-1) \\ &\quad \times \mathring{\varphi}(E, N-1) + \Delta K(n, N)\,\mathring{\varphi}(E, N); \\ &\cdots\cdots\cdots\cdots\cdots\cdots \\ \varphi(E, 0) &= \Delta K(0, 0)\,\mathring{\varphi}(E, 0) + \ldots \\ &\quad + \Delta K(0, N-1)\,\mathring{\varphi}(E, N-1) + \Delta K(0, N)\,\mathring{\varphi}(E, N). \end{aligned}\right\} \tag{27}$$

To determine the functions φ, it is now sufficient to find the coefficients $K(n, m)$.

Because of the tridiagonality of the matrix of Eqs. (26), in which V occurs only on a diagonal, and because $\varphi(E, N) = \mathring{\varphi}(E, N)$ in accordance with (21), we have $K(n, n) = 1/\Delta$.

Indeed, it is readily seen from the successive solution of the algebraic equations in (26) that the potential V never occurs in a factor of the highest power of E in the polynomials $\varphi(E, n)$, since this factor is essentially formed on the right-hand side of (26) [at the point n, it is equal to $\sqrt{2a}(-2\Delta^2)^{N-n}$]. Therefore, the coefficients of the highest powers of E in $\varphi(E, n)$ and $\mathring{\varphi}(E, n)$ are pairwise equal for all n in the interaction region, i.e., $K(n, n) = 1/\Delta$:

$$\varphi(E, n) = \mathring{\varphi}(E, n) + \sum_{m=n+1}^{N} \Delta K(n, m)\,\mathring{\varphi}(E, m). \tag{28}$$

Algebraic Analog of the Integral Equations of the Inverse Problem. The polynomials φ must be orthogonalized with respect to the energy variable in accordance with the relations (23), which are a modification of the completeness condition (14). Therefore, $K(n, m)$ in (27) can be regarded as orthogonalization coefficients of polynomials constructed from $\mathring{\varphi}$ with respect to the new measure $\rho(E)$. The $\mathring{\varphi}$ are themselves orthogonal with respect to the measure $\mathring{\rho}(E)$:

$$\int \mathring{\varphi}(E, n)\,\mathring{\varphi}(E, m)\,d\mathring{\rho}(E) = \delta_{mn}\Delta. \tag{29}$$

In order to obtain linear equations for K, it is convenient to use, not the relations (23) themselves, but the equivalent conditions of orthogonality of $\varphi(E, n)$ to all $\mathring{\varphi}(E, m)$ with $m > n$:

$$\sum_\lambda \gamma_\lambda^2 \varphi(E, n)\,\mathring{\varphi}(E, m) \equiv \int \varphi(E, n)\,\mathring{\varphi}(E, m)\,d\rho(E) = 0. \tag{30}$$

Indeed, to achieve $\varphi(E, N-1) \perp \varphi(E, N)$, we must, in accordance with the second equation in (27), ensure $\varphi(E, N-1) \perp \mathring{\varphi}(E, N)$; for $\varphi(E, N-2)$ to be orthogonal to $\varphi(E, N-1)$ and $\varphi(E, N)$, it is sufficient to make $\varphi(E, N-2)$ orthogonal to $\mathring{\varphi}(E, N-1)$ and $\mathring{\varphi}(E, N)$, from which one constructs $\varphi(E, N-1)$ and $\varphi(E, N)$, etc.

Substituting φ in the form (27) into (29), we obtain

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[5] Equation (23) can be rewritten in a different form if the sum is replaced by an integral with respect to the *spectral measure*,

$$\rho(E) = \sum_\lambda \Theta(E - E_\lambda)\gamma_\lambda^2;$$

$$d\rho(E) = \sum_\lambda \delta(E - E_\lambda)\gamma_\lambda^2\,dE, \tag{24}$$

with the step function $\Theta(x) = \{0 \text{ for } x < 1;\ 1 \text{ for } x \geq 0\}$:

$$\int \varphi(E, n)\,\varphi(E, m)\,d\rho(E) = \delta_{mn}\Delta. \tag{25}$$

[6] Matrices of this form (symmetric and tridiagonal) are called Jacobi matrices. It is interesting that we here return to the algebraic prototype of the inverse scattering problem; now, however, by virtue of the finite-difference formalism of R-matrix theory, the purely mathematical concepts take on a physical meaning: the Jacobi matrix is itself the Hamiltonian of the system, its eigenvalues are the energies of the resonances, etc.

[7] It is convenient to write the factors Δ in all sums with respect to the coordinate variable so that in the limit $\Delta \to 0$ these sums go over into corresponding integrals: $\sum_n \Delta f(n) \to \int f(r)\,dr$.

linear algebraic equations for $K(n, m)$:

$$Q(n, m) + \sum_{p=n+1}^{N} \Delta K(n, p) Q(p, m) = 0, \quad (31)$$

where

$$Q(n, m) = \sum_{\lambda} \gamma_\lambda^2 \mathring{\varphi}(E_\lambda, n) \mathring{\varphi}(E_\lambda, m). \quad (32)$$

Equations (31) play here the same role as the Gel'fand-Levitan–Marchenko integral equations in the classical inverse problem formalism (see Sec. 3). The exact algebraic analog of the latter is obtained by the slight change of the notation[8] $\overline{Q}(n, m) = Q(n, m) - \delta_{nm}/\Delta$:

$$K(n, m) + \overline{Q}(n, m) + \sum_{p=n+1}^{N} \Delta K(n, p) \overline{Q}(p, m) = 0, \quad m > n. \quad (34)$$

Thus, from the original $\{E_\lambda, \gamma_\lambda\}$ and the known $\mathring{\varphi}$ we determine $Q(n, m)$ [or $\overline{Q}(n, m)$] in accordance with (32). Then, solving (31), we find $K(n, m)$. Substituting these quantities into (27), we obtain φ. And, knowing the solution φ of the Schrödinger equation (2), we can also readily find the potential V.

Connection between V and K. We substitute φ in the form (28) into (2), multiply both sides of the equation by $\mathring{\varphi}(E, n)$, and integrate with respect to the measure $\mathring{\rho}(E)$. Taking into account (20) and (29), we obtain

$$V(n) = -[K(n, n+1) - K(n-1, n)] 2\Delta. \quad (35)$$

In the limit $\Delta \to 0$, this formula goes over into the well known expression (70) of the Gel'fand–Levitan–Marchenko theory for the connection between the potential and the kernel of the transformation of $\mathring{\varphi}$ into φ.

Comparison with the Method of Recursion Relations. A rough estimate of the increase in the number of operations (with increasing N) needed to solve the equation of the inverse problem gives a dependence proportional to N^4 (or $\sim\Delta^{-4}$) for the method of finding $V(n)$ considered here, while a dependence $\sim N^2$ is obtained for the method using the recursion relations (16) and (17). Control calculations on a computer showed that the computer times needed to find $V(n)$ (after subtraction of the translation time) increase in approximately the same proportions.[9]

We may mention in passing that, using the auxiliary functions φ and $\mathring{\varphi}$, one can obtain a further variant of the inverse problem equation with recursion relations:

$$\varphi(E_\lambda, n) = 2\Delta^2 [V(n+1) - E_\lambda + 1\ \Delta^2] \varphi(E_\lambda, n+1) - \varphi(E_\lambda, n-2); \quad (36)$$

$$V(n) = (1\ 2\Delta) \sum_{\lambda=1}^{N} \gamma_\lambda^2 \varphi(E_\lambda, n-1) \mathring{\varphi}(E_\lambda, n) - (1\ 2\Delta) \sum_{\lambda=1}^{N} \gamma_\lambda^2 \varphi(E_\lambda, n) \mathring{\varphi}(E_\lambda, n-1). \quad (37)$$

The expression (37) for $V(n)$ is obtained by multiplying (2) for $\varphi(E_\lambda, n)$ by $\gamma_\lambda^2 \mathring{\varphi}(E_\lambda, n)$, summing both sides of the equation over λ with allowance for (30), (20), and

$$\sum_{\lambda=1}^{N} \gamma_\lambda^2 \varphi(E_\lambda, n) \mathring{\varphi}(E_\lambda, n) = \sum_{\lambda=1}^{N} \gamma_\lambda^2 \varphi(E_\lambda, n) \mathring{\varphi}(E_\lambda, n) = 1\ \Delta. \quad (38)$$

which follows from (23) and (28).

The relation (37) can also be rewritten in the form

$$V(n) = [\tilde{K}(n-1, n) - \tilde{K}(n, n-1)] 2\Delta, \quad (39)$$

where

$$\tilde{K}(n, m) = (1\ \Delta) \sum_{\lambda} \gamma_\lambda^2 \varphi(E_\lambda, n) \mathring{\varphi}(E_\lambda, m) \quad (40)$$

are the coefficients of the transformation from $\mathring{\varphi}$ to φ [the inverse of (27)]. Thus, $\tilde{K}(n, n-1)$ ($n = N, N-1, \ldots, 1$), which are the neighbors of the diagonal $K(n, n) = 1/\Delta$, can be found by means of the recursion relations (36), (39), and (40). The continuous analog of this procedure is obtained by successive differentiation of the transformation from φ to $\mathring{\varphi}$: $\mathring{\varphi} = \varphi + \int_r^a \tilde{K} \varphi\, dr'$ and its kernel $\tilde{K}(r, r') = \int \varphi(E, r) \mathring{\varphi}(E, r') d(\rho - \mathring{\rho})$. As a result $(d^n/dr^n) V(r)|_{r=a}$ is calculated, and from it $V(r)$ is determined in the region of convergence of the Taylor series for the potential.

Velocity-Dependent Potentials. In nuclear physics, to take into account effectively the repulsion of particles at short distances, use is sometimes made of an interaction of the type

$$V(p) = V_0(r) + [p^2 V_1(r) 2 + V_1(r) p^2 2] 2. \quad (41)$$

where $p = -i\nabla$ is the momentum operator. Such a potential leads to the appearance in the Schrödinger equation of a variable coefficient, which depends on the coordinate r, in front of the kinetic energy operator (the second derivative). In the finite-difference approximation, this Schrödinger equation has the form[10]

$$\begin{aligned} &-\{\Psi(E, n+1) - 2\Psi(E, n) + \Psi(E, n-1)\} \\ &+ \{1 + V_1(n)\ 2\}\ 2\Delta^2 + V_0(n)\ \Psi(E, n) \\ &-\{V_1(n+1)\ \Psi(E, n+1) - 2V_1(n) \Psi(E, n) \\ &+ V_1(n-1)\ \Psi(E, n-1)\}\ 4\Delta^2 = E\ \Psi(E, n). \end{aligned} \quad (42)$$

[8] The coefficients $\overline{Q}$ can be represented in the form

$$\overline{Q}(n, m) = \int \mathring{\varphi}(E, n) \mathring{\varphi}(E, m)\, d[\rho(E) - \mathring{\rho}(E)]. \quad (33)$$

[9] The expression (35) for the potential can be obtained from (17) by substituting into the latter $u_\lambda(n) = \gamma_\lambda \varphi(E, n)$ and $\varphi(E_\lambda, n)$ in the form (28) with allowance for (20) and (30) and the equation $K(n, n-1) = (1/\Delta) \int \varphi(E, n) \varphi(E, n-1) d\rho$, which follows from (27).

[10] In the derivation of (42), one must bear in mind the specific nature of finite-difference differentiation of a product[23] ("spreading" of the arguments). We denote the operators of right and left finite-difference differentiation by $\delta_\pm$:

$$\delta_- f(n) = [f(n-1) - f(n)]\ \Delta;$$
$$\delta_+ f(n) = [f(n) - f(n+1)]\ \Delta.$$

Then $\delta_-[f(n) g(n)] = f(n-1)\, \delta_- g(n) + g(n)\, \delta_- f(n)$;

$$\delta_+[f(n)\, g(n)] = f(n-1)\, \delta_+ g(n) + g(n)\, \delta_+ f(n).$$

The second derivative has the form

$$\delta_+ \delta_- [f(n)\ g(n)] = \{f(n+1)\, g(n-1) - 2g(n)\, f(n) + g(n-1)\, f(n-1)\}\ \Delta^2 = \delta_- \delta_+ [f(n)\, g(n)].$$

We shall, as above, assume that the forces have a finite range $V_0(r \geq a) = V_1(r \geq a) = 0$ (or that V_0 and V_1 are known for $r > a$). As in the case of an ordinary potential, the solutions $u(E_\lambda, n) \equiv u_\lambda(n)$ satisfying the homogeneous boundary conditions (12) form a complete orthonormal set: Equations (13) and (14) are satisfied (the proof is along the same lines as in Appendix 2). The relations (27), (29), (30) and (32) also remain true. The orthogonalization coefficients are found, not from (31), but from the system of equations

$$\Delta K(n, n) Q(n, m) - \sum_{p=n-1}^{N} \Delta K(n, p) Q(p, m) = 0, \quad n > m;$$
$$Q(n, n) - \sum_{p=n-1} K(n, p) Q(p, n) K^{-1}(n, n) = K^{-2}(n, n) \Delta^3.$$

where there is an additional equation for $K(n, n)$ obtained by substituting (27) into (23) for $n = m$. This slight complication of the system of equations for K is due to the fact that in the case of the potential $V(\hat{p}^2)$ the coefficients of the highest powers of E in the polynomials $\mathring{\varphi}(E, n)$ and $\varphi(E, n)$ are no longer equal, i.e., $K(n, n) \neq 1/\Delta$.

The connection between V and K is determined, not by (35), but by the recursion relations

$$V_1(n-1) = 2K(n, n) K(n-1, n-1) - 2 - V_1(n);$$
$$V_0(n) = -(1/2\Delta^2)[K(n, n-1) K(n, n) - K(n-1, n) K(n-1, n-1)] - V_1(n) \Delta^2. \quad (43)$$

The first equation in (43) is obtained by multiplying (42) for $\varphi(E, n)$ by $\mathring{\varphi}(E, n-1)$ and integrating with respect to δ using (27). The second equation in (43) is obtained by multiplying (42) for $\varphi(E, n)$ by $\mathring{\varphi}(E, n)$ and integrating with respect to δ with allowance for (27).

In Ref. 15, other recursion relations are given:

$$V_1(n-1) = -[1/2\Delta^2 - V_1(n)] 4\Delta^2 - H_{n, n-1}] 4\Delta^2;$$
$$V_0(n) = H_{nn} - 1/\Delta^2 - V_1(n)/\Delta^2, \quad (44)$$

where

$$H_{nn} = \sum_\lambda E_\lambda \gamma_\lambda^2 \mathring{q}(E_\lambda, n) \mathring{q}(E_\lambda, m).$$

The solution of this inverse problem for velocity-dependent potentials may be of interest for constructing a finite-difference Hamiltonian which is *phase-equivalent* to the differential operator[11] corresponding to Eq. (1). The point is that although a finite-difference potential $V(n)$ giving the same scattering parameters as $V(r)$ does not exist in the general case, one can always find a finite-difference potential $V(\hat{p}^2)$ corresponding to it. However, it has not yet been investigated how close such a finite-difference potential $V(\hat{p}^2)$ is to $V(r)$; is the "perturbation" $V_1(n)$ and $V_0(n) - V(r_n)$ large?

Gel'fand-Levitan finite-difference method

Since the formalism of the inverse problem in finite-difference R-matrix theory[6,16] presented above is similar to the finite-difference analog of the Gel'fand–Levitan method,[4] we shall not dwell in detail on the latter. We shall merely point out various aspects that distinguish this approach in the case of a finite-range potential from its R-matrix modification.

The auxiliary functions $\varphi(E, n)$ and $\mathring{\varphi}(E, m)$ are specified by boundary conditions, not at the point N, but at the origin:

$$q(E, 0) = \mathring{q}(E, 0) = 0; \quad q(E, 1) = \mathring{q}(E, 1) = \Delta. \quad (45)$$

The functions $\varphi(E, n)$ and $\mathring{\varphi}(E, n)$ are also polynomials in E, not of degree $n-1$, but $N-n$ (the degree of the polynomial increases as one moves away from the point $n = 1$). As eigenfunctions, the same functions $u_\lambda(n)$ as above [see (12)–(14)] can be used. Then the spectral function associated with the scattering data will be determined by E_λ and the values of $u_\lambda(1)$, and not $u_\lambda(N)$. The connection between φ and $\mathring{\varphi}$ is given, not by (27), but by the relations

$$q(E, n) = \mathring{q}(E, n) - \sum_{m=1}^{n-1} \Delta K(n, m) \mathring{q}(E, m). \quad (46)$$

As in (30), $\varphi(E, n) \perp \mathring{\varphi}(E, m)$ but here for $m < n$. The equations for $K(n, m)$, the analog of the Gel'fand–Levitan equations, and the formula relating the potential to $K(n, m)$ are similar to (31) and (35):

$$\left.\begin{aligned} &K(n, m) - \overline{Q}(n, m) - \sum_{p=1}^{n-1} \Delta K(n, p) \overline{Q}(p, m) = 0; \\ &\overline{Q}(n, m) = \sum_\lambda \Delta u_\lambda(1) \mathring{q}(E_\lambda, n) \mathring{q}(E_\lambda, m) - \delta_{mn} \Delta; \\ &V(n) = [K(n-1, n) - K(n, n-1)]/2\Delta. \end{aligned}\right| \quad (47)$$

Algebraic analog of Marchenko's method (Ref. 5)

Instead of the auxiliary solutions φ and $\mathring{\varphi}$, Marchenko's method uses the solutions $\varphi_\pm$ and $\mathring{\varphi}_\pm$ with asymptotic behavior corresponding to free waves $\exp(\pm ikr)$ in the limit $\Delta \to 0$. In this approach, $\varphi_\pm$ are related in a simple manner to the physical wave function:

$$\Psi(E, n) = A[q_-(E, n) - S(E) q_-(E, n)], \quad (48)$$

and in it Ψ and V are found from S without the intermediate introduction of a spectral function.

In the derivation of the transformation (27) from $\mathring{\varphi}$ to φ, use was made of the polynomial dependence of these functions on the energy and the fact that the number of terms with different powers of E in these polynomials increases at each step in the progression from the point N into the interaction region. Here, an analogous role is played by the polynomial dependence of $\varphi_\pm$ and $\mathring{\varphi}_\pm$ on on the new variable $z^{\pm 1}$, which is related to E.

The finite-difference analogs of $\exp(\pm ikr)$ are[5] the solutions $\mathring{\varphi}_\pm$ of Eq. (20):

$$\mathring{q}_\pm(z, n) = z^{\pm n}, \quad (49)$$

where $z \equiv \lambda - \sqrt{\lambda^2 - 1}$, and $\lambda \equiv 1 - E\Delta^2 \equiv (z + 1/z)/2$.

To see this, we note that, on the one hand, $\mathring{\varphi}_\pm$ satisfy (20), which is readily seen by rewriting the free finite-difference Schrödinger equation (20) in the form

[11] As is shown in Berezanskiĭ's book Ref. 20 (p. 525 of the Russian original), any spectral function $\rho(E)$ satisfying the condition $\int d\rho(E) = 1$, corresponds uniquely to the finite-difference expression on the left-hand side in (42).

$$\mathring{\varphi}_{\pm}(z,\ n+1)+\mathring{\varphi}_{\pm}(z,\ n-1)=(z+1/z)\,\mathring{\varphi}_{\pm}(z,\ n). \tag{20a}$$

On the other hand, since the parameter λ varies in the range $-1\leqslant\lambda\leqslant 1$ as E varies in the energy range $0\leqslant E\leqslant 2/\Delta^2$, one can set $\lambda=\cos\theta$; $z=\lambda-\sqrt{\lambda^2-1}=\cos\theta-i\sin\theta=\exp(-i\theta)$, i.e., $\sin^2\theta/2=k^2\Delta^2/4$. But in accordance with the relation $\lambda\equiv 1-E\Delta^2\equiv 1-k^2\Delta^2/2=\cos\theta$, we have

$$z^{\pm n}\xrightarrow[\substack{\Delta\to 0\\ \Delta n\to r}}\exp(\pm ikr). \tag{49a}$$

As before, we shall assume, to simplify the arguments, that there are no bound states and $V(n\geqslant N)=0$. At the points $n=N+1,\ N$, by the definition (49),

$$\varphi_{\pm}(z,\ N+1)=\mathring{\varphi}_{\pm}(z,\ N+1)=z^{\pm(N+1)}; \tag{50}$$

$$\varphi_{\pm}(z,\ N)=\mathring{\varphi}_{\pm}(z,\ N)=z^{\pm N}. \tag{51}$$

We now write the Schrödinger equation (2) in the matrix form [cf (26)]

$$\begin{pmatrix}
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & 1 & 0 & 1 & 0 & 0 & \cdots & \cdots & \cdots & \cdots \\
\cdots & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & 1 & -2\Gamma(N-1)\Delta^2 & 1 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & 1 & -2\Gamma(N-2)\Delta^2 & 1 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & 0 & 1 & -2\Gamma(N-3)\Delta^2 & 1 & 0 & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots
\end{pmatrix}$$

$$\times\begin{pmatrix}
\vdots \\
\varphi_{\pm}(z,\ N-1)=z^{\pm(N-1)} \\
\varphi_{\pm}(z,\ N)=z^{\pm N} \\
\varphi_{\pm}(z,\ N-1) \\
\varphi_{\pm}(z,\ N-2) \\
\varphi_{\pm}(z,\ N-3) \\
\vdots \\
\vdots \\
\vdots
\end{pmatrix}=\left(z+\frac{1}{z}\right)\begin{pmatrix}
\vdots \\
\varphi_{\pm}(z,\ N)=z^{\pm N} \\
\varphi_{\pm}(z,\ N-1) \\
\varphi_{\pm}(z,\ N-2) \\
\varphi_{\pm}(z,\ N-3) \\
\vdots \\
\vdots \\
\vdots
\end{pmatrix}. \tag{52}$$

This is a system of algebraic equations with *tridiagonal* coefficient matrix. From the equation that relates the known $\varphi_{\pm}(z, N+1)$ and $\varphi_{\pm}(z, N)$ to $\varphi_{\pm}(z, N-1)$, we find that $\varphi_{\pm}(z, N-1)=z^{\pm(N-1)}$. From the following equation in (52), it can be seen that $\varphi_{\pm}(z, N-2)$ contains besides $z^{\pm(N-2)}$ a further term with $z^{\pm(N-1)}$. Proceeding further, we obtain for $\varphi(z, N-3)$ a polynomial containing $z^{\pm(N-3)}$, $z^{\pm(N-2)}$, $z^{\pm(N-1)}$, $z^{\pm N}$. In each subsequent step, the number of terms with different powers of $z^{\pm 1}$ in the polynomials $\varphi_{\pm}(z, N-n)$ increases by two because of the appearance of the terms with $z^{\pm(N-n)}$ and $z^{\pm(2N-n-3)}$.

Thus, $\varphi_{\pm}$ can be constructed like (27) in the form of a linear combination of known $\mathring{\varphi}_{\pm}(z, m)=z^{\pm m}$:

$$\varphi_{\pm}(z,\ n)=\mathring{\varphi}_{\pm}(z,\ n)+\sum_{m=n+1\leqslant 2N-n-3}^{2N-n-3}\Delta K(n,\ m)\,\mathring{\varphi}_{\pm}(z,\ m), \tag{53}$$

where $K(n, m)$ guarantees that the coefficients of $z^{\pm m}$ on the two sides are equal.

From the auxiliary functions $\varphi_{\pm}$, we construct the wave function Ψ:

$$\Psi(E,\ n)=\Psi(z,\ n)=A[\varphi_{-}(z,\ n)-S(E)\varphi_{+}(z,\ n)]. \tag{54}$$

In accordance with (53), Ψ can also be represented as a linear combination of the free solutions $\mathring{\Psi}=A(\mathring{\varphi}_{-}-S\mathring{\varphi}_{+})$:

$$\Psi(z,\ n)=\mathring{\Psi}(z,\ n)+\sum_{m=n-1\leqslant 2N-n-3}^{2N-n-3}\Delta K(n,\ m)\,\mathring{\Psi}(z,\ m), \tag{55}$$

where

$$\mathring{\Psi}(z,\ n)=\mathring{\varphi}_{-}(z,\ n)-S(E)\,\mathring{\varphi}_{+}(z,\ n)=A(z^{-n}-Sz^{+n}).$$

We find the coefficients K by means of the completeness condition (orthogonality with respect to E) for the wave functions normalized in accordance with (54):

$$\frac{1}{2\pi}\int_0^{2/\Delta^2}\Psi(E,\ n)\,\Psi^{*}(E,\ m)\,dE$$

$$=\frac{1}{2\pi i}\oint\Psi(z,\ n)\,\Psi^{-}(z,\ m)\frac{dz}{\Delta A^2 z}=\frac{\delta_{mn}}{\Delta}, \tag{56}$$

where the contour of integration is the circle of unit radius. In accordance with (55), it follows from (56) that $\Psi(E, n)$ is orthogonal (with respect to E) to all $\mathring{\Psi}(E, m)$ with $m>n$ [cf (30)]:

$$\frac{1}{2\pi}\int_0^{2/\Delta^2}\Psi(E,\ n)\,\mathring{\Psi}^{-}(E,\ m)\,dE=\frac{1}{2\pi i}\oint\Psi(z,\ n)$$

$$\times\mathring{\Psi}^{+}(z,\ m)\frac{dz}{\Delta A^2 z}=0\quad\text{for } m>n. \tag{57}$$

Substituting Ψ in the form (55) into (57), we obtain a system of linear equations for K:

$$K(n,\ m)+\overline{F}(n,\ m)+\sum_{p=n+1\leqslant 2N-n-3}^{2N-n-3}\Delta K(n,p)\,\overline{F}(p,m)=0, \tag{58}$$

where

$$\overline{F}(n,\ m)=F(n+m)-\frac{\delta_{mn}}{\Delta}=\frac{1}{2\pi i}\int_0^{r,\Delta^2}\mathring{\Psi}(z,\ n)\,\mathring{\Psi}^{+}(z,\ m)$$

$$\times\frac{dz}{\Delta A^2 z}-\frac{\delta_{mn}}{\Delta}=\frac{1}{2\pi i}\oint(1-S(z))\,z^{n+m}\frac{dz}{\Delta A^2 z}-\frac{\delta_{mn}}{\Delta}. \tag{59}$$

Equation (58) is the algebraic analog of the integral equation of Marchenko's method.

The required potential is related to K by the usual [cf (35)] relation (derived in Appendix 3):

$$V(n)=-[K(n,\ n+1)-K(n-1,\ n)]/2\Delta. \tag{60}$$

3. INVERSE SCATTERING PROBLEM (FOR $\Delta=0$)

Now that we know the finite-difference formalism of the inverse problem, the transition to a continuous coordinate dependence must seem almost trivial. As an example, we give the variant of the inverse problem in the framework of R-matrix scattering theory. The Gel'fand–Levitan and Marchenko methods (for $\Delta=0$) have been frequently and extensively studied in the literature[1-3,8-12] and it would be inappropriate to repeat them here.

For simplified orientation among the various inverse problem methods, we emphasize once more the *universality* of the procedure for orthogonalization (through the

completeness property) of the solutions of the Schrödinger equation when they are constructed from known functions. It is interesting that even the inverse problem method at fixed energy can be regarded as one of these methods, although it is usually expounded without apparent connection with them.

Finding of the Potential from E_λ and λ_λ. We give here the basic formulas of the method, referring to the corresponding finite-difference relations. The eigenfunctions $u(E_\lambda r) \equiv u_\lambda(r)$ corresponding to boundary conditions at $r=0$ and $r=a$ [cf (12)]:

$$u_\lambda(0)=0; \quad u'_\lambda(a)/u_\lambda(a)=B/a, \tag{61}$$

form an *infinite* discrete orthonormal complete set [cf (13) and (14)]:

$$\int_0^a u_\lambda(r)\,u_{\lambda'}(r)\,dr=\delta_{\lambda\lambda'}; \quad (\lambda, \lambda'=1, 2 \ldots \infty); \tag{62}$$

$$\sum_{\lambda=1}^{\infty} u_\lambda(r)\,u_\lambda(r')=\delta(r-r'). \tag{63}$$

For the auxiliary solutions φ and $\mathring{\varphi}$ of the Schrödinger equation (1), the following boundary conditions are chosen [cf (21)]:

$$\left.\begin{aligned} &\varphi(E, a)=\mathring{\varphi}(E, a)=\sqrt{2a}; \\ &\varphi'(E, a)\,\varphi(E, a)=\mathring{\varphi}'(E, a)\,\mathring{\varphi}(E, a)=B\,a. \end{aligned}\right\} \tag{64}$$

As in the finite-difference case, $u_\lambda(r)=\varphi(E_\lambda, r)\gamma_\lambda$, and, in accordance with (63) [cf (23) and (25)]

$$\sum_{\lambda=1}^{\infty} \varphi(E_\lambda, r)\,\varphi(E_\lambda, r')\,\gamma_\lambda^2 \equiv \int_{-\infty}^{\infty} \varphi(E, r)\,\varphi(E, r')\,d\rho(E)=\delta(r-r'). \tag{65}$$

The solutions φ and $\mathring{\varphi}$ are related as in (28):

$$\varphi(E, r)=\mathring{\varphi}(E, r)+\int_r^a K(r, r')\,\mathring{\varphi}(E, r')\,dr'. \tag{66}$$

For the kernel $K(r, r')$ we obtain the Gel'fand–Levitan–Marchenko equations, orthogonalizing φ with respect to the measure $\rho(E)=\sum_{\lambda=1}^{\infty}\Theta(E-E_\lambda)\gamma_\lambda^2$, or from the equivalent requirement [cf (30)]:

$$\int \varphi(E, r)\,\mathring{\varphi}(E, r')\,d\rho(E)=0 \quad \text{for } r'>r. \tag{67}$$

Substituting (66) into (67), we obtain [cf (34)]

$$K(r, r')+Q(r, r')+\int_r^a K(r, r'')\,Q(r'', r')\,dr''=0, \tag{68}$$

where [cf (32)]

$$Q(r, r')=\int \mathring{\varphi}(E, r)\,\mathring{\varphi}(E, r')\,d[\rho(E)-\mathring{\rho}(E)]. \tag{69}$$

The required potential is determined by the derivative of the kernel $K(r, r')$ at equal arguments [cf (35)]:

$$V(r)=-\frac{d}{dr}K(r, r'). \tag{70}$$

Complex (Optical) Potential. If the required potential has an imaginary component $\mathrm{Im}\,V(r)\neq 0$, the operator corresponding to the Schrödinger equation with boundary conditions (61) is no longer self-adjoint. The orthogonality and completeness conditions are no longer satisfied for the eigenfunctions $u_\lambda(r)$. However, instead of orthogonality with respect to the coordinate and energy variables, one must use *biorthogonality*[12)] of the sets $\{u_\lambda(r)\}$ and $\{u_\lambda^*(r)\}$. Because $[u_\lambda^*(r)]^*=u_\lambda(r)$, the form of Eqs. (62)–(70) does not change when $V(r)$ ceases to be real; it is only necessary to remember that $[\varphi(E, r), \mathring{\varphi}(E, r), u_\lambda(r), E_\lambda, \gamma_\lambda, K(r, r'), Q(r, r')]$ in them become complex.

Inverse Problem for $E=const$. The inverse problem formalism for $E=\mathrm{const}$[10] is usually presented in a different way from the case $l=\mathrm{const}$. However, a unified approach is possible. As was shown in Ref. 18, the solutions of the Schrödinger equation with continuously varying orbital angular momentum l but fixed energy E form a complete set (see also Ref. 34). The corresponding Parseval equation has the form [cf (65)]:

$$\int \frac{f(\lambda, -k, r)}{r}\,\frac{f(\lambda, -k, r')}{r}\,d\rho_k(\lambda)=\delta(r-r'), \tag{71}$$

where $\lambda \equiv l-\frac{1}{2}$; f is the solution of the Jost equation

$$\begin{aligned} &-f''(\lambda, \pm k, r)+(\lambda^2-1/4)\,f(\lambda, \pm k, r)/r^2 \\ &\quad +V(r)\,f(\lambda, \pm k, r)=k^2 f(\lambda, \pm k, r) \end{aligned} \tag{72}$$

satisfying the asymptotic condition $\lim_{r\to\infty} f\exp(\pm i kr)=1$, and $\rho_k(\lambda)$ is the spectral function.

One can write down the connection between f and the corresponding solutions $\mathring{f}$ of Eq. (72) with $V=0$ [cf (66)]:

$$\frac{f(\lambda, -k, r)}{r}=\frac{\mathring{f}(\lambda, -k, r)}{r}+\int_r^{\infty}\frac{K_k(r, r')}{r}\,\frac{\mathring{f}(\lambda, -k, r')}{r'}\,dr'. \tag{73}$$

The integral equation for K_k has the form [cf (68)]:

$$\frac{K_k(r, r')}{r}+\frac{Q(k, r, r')}{r'}+\int_r^{\infty}\frac{K_k(r, r'')}{r}\,\frac{Q(k, r'', r')}{r'}\,dr''=0, \tag{74}$$

where [cf (69)]

$$\frac{Q(k, r, r')}{r'}=\int \frac{\mathring{f}(\lambda, -k, r)}{r}\,\frac{\mathring{f}(\lambda, -k, r')}{r'}\,d[\rho_k(\lambda)-\mathring{\rho}_k(\lambda)], \tag{75}$$

and for the required potential

$$V(r)=-\frac{d}{dr}K(r, r'). \tag{76}$$

Thus, the potential can be found from the spectral function $\rho_k(\lambda)$, which is determined by the scattering matrix S, which depends on the continuous variable l.

Since the experiment provides the values of S_l only for integral l, there exists a family of potentials corresponding to different ways of extending S_l to the complete l axis (for fixed energy E).

[12)] In the case of relativistic equations, *quasiorthogonality* is also used.[17]

4. DETERMINATION OF THE INTERACTION IN THE MANY-CHANNEL CASE

The equations of motion for coupled channels have the form ($\hbar = 1$, $m = 1$):

$$-(1/2)F_\alpha''(E, r) + \sum_{\alpha'} V_{\alpha\alpha'}(r) F_{\alpha'}(E, r) = EF_\alpha(E, r); \tag{77}$$

here, $F_\alpha(E, r)$ are the channel wave functions forming the vector solution $F(E, r) \equiv \{F_1(E, r), F_2(E, r) \ldots\}$; $V_{\alpha\alpha'}(r)$ is the matrix of the interaction that couples the channels. In the general case, $E_\alpha F_\alpha$ occurs on the right-hand side of (77). The corresponding inverse problem is considered below. The finite-difference analog of (77) is the system of algebraic equations

$$-\frac{1}{2\Delta^2}\{F_\alpha(E, n+1) - 2F_\alpha(E, n) + F_\alpha(E, n-1)\} + \sum_{\alpha'} V_{\alpha\alpha'}(n) F_{\alpha'}(E, n) = E_\alpha F_\alpha(E, n). \tag{78}$$

We shall assume that the range of $V_{\alpha\alpha'}$ is bounded $[V_{\alpha\alpha'}(n \geq N) = 0]$, and the number of channels finite ($\alpha = 1, 2, \ldots, M$). As basis functions, we choose vector eigenfunctions $u_{\alpha\lambda}(n)$ satisfying homogeneous boundary conditions of the type (12):

$$u_\alpha(E, 0) = 0; \quad u_\alpha(E, N-1) = u_\alpha(E, N)(1 + B_\alpha\Delta/a). \tag{79}$$

Together with (78), they give a system of $N \times M$ homogeneous algebraic equations for $u_\alpha(E, n)$ ($\alpha = 1, 2, \ldots, M$; $n = 1, 2, \ldots, N$). This system has solutions for $N \times M$ values of the energy $E = E_\lambda$ ($\lambda = 1, 2, \ldots, N \times M$), which form an orthonormal complete set of vector functions $u(E_\lambda, n) \equiv u_\lambda(n) = \{u_{1\lambda}(n), u_{2\lambda}(n), \ldots\}$:

$$\sum_{\alpha=1}^{M}\sum_{n=1}^{N} \Delta u_{\alpha\lambda}(n) u_{\alpha\lambda'}(n) = \delta_{\lambda\lambda'}; \tag{80}$$

$$\sum_{\lambda=1}^{N\times M} u_{\alpha\lambda}(n) u_{\beta\lambda}(m) = \delta_{mn}\delta_{\alpha\beta}/\Delta. \tag{81}$$

These relations are derived in Appendix 2.

For comparison of the relations (14) and (15) in the single-channel case with (80) and (81), let us consider the example of two channels ($M = 2$) in the limit of no coupling between them: $V_{12}(n) \equiv V_{21}(n) \equiv 0$. Then (78) decomposes into two independent systems of equations for $F_1(E, n)$ and $F_2(E, n)$. Together with the boundary conditions (79), we have two individual systems, each with N homogeneous algebraic equations for $u_1(E, n)$ and $u_2(E, n)$ of the type (13): one for each channel. One of them has solutions for $E = E_{1\lambda_1}(\lambda_1 = 1, 2, \ldots, N)$, and the other for $E = E_{2\lambda_2}(\lambda_2 = 1, 2, \ldots, N)$. The solutions of each of them form a complete orthonormal set in the space of finite-difference functions in the interval $0 < n \leq N$ like (14) and (15) [cf (80) and (81)]:

$$\left.\begin{aligned} \sum_{n}^{N} \Delta u_{\alpha\lambda_\alpha}(n) u_{\alpha\lambda'_\alpha}(n) &= \delta_{\lambda_\alpha\lambda'_\alpha} \\ \sum_{\lambda_\alpha}^{N} u_{\alpha\lambda_\alpha}(n) u_{\alpha\lambda_\alpha}(m) &= \delta_{mn}/\Delta \end{aligned}\right\} \text{for } \alpha = 1, 2. \tag{82}$$

At the same time, $u_{1\lambda_1}(n)$ and $u_{2\lambda_2}(n)$ together form a complete orthonormal set in the space of vector functions:

$$\begin{pmatrix} u_{1\lambda}(n) \\ u_{2\lambda}(n) = 0 \end{pmatrix} (\lambda = \lambda_1 = 1, 2 \ldots N)$$

and

$$\begin{pmatrix} u_{1\lambda}(n) = 0 \\ u_{2\lambda}(n) \end{pmatrix} (\lambda = \lambda_2 + N = N-1, N-2 \ldots 2N)$$

and they satisfy the relations (80) and (81).

The values of the eigenfunctions on the boundary $u_{\alpha\lambda}(N) \equiv \gamma_{\alpha\lambda}\sqrt{2a}$ are the partial reduced widths, and the E_λ, the positions of the resonances of the R-matrix, form the set of scattering parameters that determine the R-matrix (see the derivation in Appendix 1):

$$R_{\alpha\alpha'}(E) = \sum_{\lambda} [\gamma_{\alpha\lambda}\gamma_{\alpha'\lambda}/(E_\lambda - E)]. \tag{83}$$

In the many-channel case, the inverse problem can be formulated as follows: Find $V_{\alpha\alpha'}(n)$ from the set

$$\{\gamma_{\alpha\lambda}, E_\lambda\} \quad (\alpha = 1, 2 \ldots M, \ \lambda = 1, 2 \ldots N \times M). \tag{84}$$

Recursions Relations. From the system of many-channel equations (78) and the completeness conditions (81), a matrix generalization of the recursion relations (17) and (18) is obtained:

$$u_{\alpha\lambda}(n) = 2\Delta^2 \sum_{\alpha'=1}^{M} V_{\alpha\alpha'}(n+1) u_{\alpha\lambda}(n+1) + 2(1 - \Delta^2 E_\lambda) u_{\alpha\lambda}(n+1) - u_{\alpha\lambda}(n+2); \tag{85}$$

$$V_{\alpha\alpha'}(n) = \Delta \sum_{\lambda=1}^{N\times M} E_\lambda u_{\alpha\lambda}(n) u_{\alpha'\lambda}(n) - \delta_{\alpha\alpha'}/\Delta^2. \tag{86}$$

The number of operations which must be performed to solve the many-channel inverse problem by means of (85) and (86) increases with M and N as $M^3 \times N^2$.

To satisfy the boundary conditions at the two ends of the interval of integration in the direct problem, it is necessary to solve the system of many-channel equations M times (with linearly independent boundary conditions at one point) and construct the required solution from the resulting auxiliary solutions.[19] In the inverse problem, the solution is obtained in a single "run."

Determination of the Original Potential from $V_{\alpha\alpha'}$. If $V_{\alpha\alpha'}(r)$ are the matrix elements of the potential energy $V(r, \xi)$ between the functions of some known basis set $\{\Phi_\alpha(\xi)\}$:

$$V_{\alpha\alpha'}(r) = \int \Phi_\alpha^*(\xi) V(r, \xi) \Phi_{\alpha'}(\xi) d\xi, \tag{87}$$

it is of interest to determine $V(r, \xi)$ from the $V_{\alpha\alpha'}(r)$ found in the inverse problem. Assuming that the set $\{\Phi_\alpha(\xi)\}$ is orthonormal and complete, the connection can be readily established. Indeed, the $V_{\alpha\alpha'}(r)$ are the coefficients of the expansion of the product $V(r, \xi)\Phi_{\alpha'}(\xi)$ in a series with respect to $\Phi_\alpha(\xi)$:

$$V(r, \xi)\Phi_\alpha(\xi) = \sum_{\alpha'} V_{\alpha\alpha'}(r)\Phi_{\alpha'}(\xi). \tag{88}$$

In their turn, the values of $V\Phi_\alpha$ determine the coeffi-

cients of the expansion of $V(r, \xi)$ with respect to Φ_α:

$$V(r, \xi) = \sum_{\alpha'} \left\{ \int V(r, \xi) \Phi^*_{\alpha'}(\xi') d\xi \right\} \Phi_{\alpha'}(\xi). \quad (89)$$

Substituting (88) into (89), we obtain

$$V(r, \xi) = \sum_{\alpha'} C_{\alpha'}(r) \Phi_{\alpha'}(\xi), \quad (90)$$

where

$$C_{\alpha'}(r) = \sum_{\alpha''} V_{\alpha'\alpha''}(r) \int \Phi_{\alpha''}(\xi') d\xi'. \quad (91)$$

Our arguments and (87)–(91) are true in the case of continuous and discrete values of the coordinate variable r.

Solution of the Inverse Problem by the Orthogonalization Method. In the many-channel case, the matrices of the solutions $\Phi(E, n) = \|\varphi_{\alpha\beta}(E, n)\|$ play the role of the auxiliary functions, the polynomials φ (and $\mathring{\varphi}$). Each vector column of Φ is a solution of the system (78) with inhomogeneous boundary conditions at $r = a$[cf (21)]:

$$\varphi_{\alpha\beta}(E, N) = \delta_{\alpha\beta}\sqrt{2a};$$
$$\varphi_{\alpha\beta}(E, N+1) = \varphi_{\alpha\beta}(E, N)(1 + B_\alpha \Delta \delta_{\alpha\beta}/a). \quad (92)$$

Like (22), the vector eigenfunctions $\{u_{\alpha\lambda}(n)\}$ can be obtained by multiplying the matrix Φ by the vector of the partial widths $\{u_{\alpha\lambda}(N)\} \equiv \{\gamma_{\alpha\lambda}\sqrt{2a}\}$ (the order of multiplication is now important):

$$u_{\beta\lambda}(n) = \sum_\alpha \varphi_{\beta\alpha}(E_\lambda, n) \gamma_{\alpha\lambda}. \quad (93)$$

Substituting (93) into the completeness condition for the eigenfunctions (81), we obtain relations for orthonormalization of $\varphi_{\alpha\beta}$ as functions of the energy with a spectral function weight that is the matrix $\rho_{\alpha\beta} = \sum_\lambda \Theta(E - E_\lambda)\gamma_{\alpha\lambda}\gamma_{\beta\lambda}$:

$$\sum_{\lambda\delta\eta} \varphi_{\alpha\delta}(E_\lambda, n) \gamma_{\delta\lambda}\gamma_{\eta\lambda}\varphi_{\eta\beta}(E_\lambda, m) = \delta_{mn}\delta_{\alpha\beta}\Delta. \quad (94)$$

The polynomial dependence of $\varphi_{\alpha\beta}$ on the energy can be proved in the same way as in the single-channel problem, except that now the coefficient matrix of the system (78) is not simply tridiagonal, as in (26), but *block-tridiagonal.* To each matrix element in (26) there now corresponds a matrix with indices of the channels: $\|V_{\alpha\beta}(n)\|$ instead of $V(n)$; $\hat{I}(1/\Delta^2)$ instead of $1/\Delta^2$, etc. Therefore, $\Phi(E, n) = \|\varphi_{\alpha\beta}\|$ and $\mathring{\Phi}(E, n) = \|\mathring{\varphi}_{\alpha\beta}\|$ are polynomials in E, but with matrix coefficients. Because of this, we can seek Φ in the form of linear combinations of Φ analogous to (27) and (28):

$$\varphi_{\alpha\beta}(E, n) = \mathring{\varphi}_{\alpha\beta}(E, n) + \sum_{n'=n}^{N} \Delta \sum_\delta K_{\alpha\delta}(n, n') \mathring{\varphi}_{\delta\beta}(E, n'). \quad (95)$$

For the coefficients K, we obtain the system of equations [see (31) and (34)]

$$K_{\alpha\beta}(n, n') + \overline{Q}_{\alpha\beta}(n, n') + \sum_{p=n+1}^{N} \Delta \sum_\delta K_{\alpha\delta}(n, p) \overline{Q}_{\delta\beta}(p, n') = 0, \quad (96)$$

where

$$\overline{Q}_{\alpha\beta}(n, n') = \sum_\lambda \mathring{\varphi}_{\alpha\alpha}(E_\lambda, n) \gamma_{\alpha\lambda}\gamma_{\beta\lambda}\mathring{\varphi}_{\beta\beta}(E_\lambda, n') - \delta_{nn'}\delta_{\alpha\beta}/\Delta. \quad (97)$$

As in the single-channel case, a connection between the required interaction matrix and K can be derived:

$$V_{\alpha\beta}(n) = -\frac{1}{2\Delta}\{K_{\alpha\beta}(n, n+1), \; -K_{\alpha\beta}(n-1, n)\}. \quad (98)$$

5. MULTIDIMENSIONAL PROBLEMS

Systems with interaction V that depends on several variables are, it is true, difficult, but nevertheless very interesting for investigation. If V has no symmetry, the variables in the Schrödinger equation do not separate, and the partial differential equation has infinitely many linearly independent solutions at each energy instead of the two for the one-dimensional equation of motion.

The most promising application seems to be to use the multidimensional inverse problem to determine the minimum of experimental information needed to establish V and to find the connections between scattering data.

In the case of the qualitatively more complicated multidimensional theory, it is particularly expedient to consider first discrete variants of the inverse problem.

Finite-Difference Schrödinger Equation. To get a feeling for the multidimensional problems, two dimensions are fully adequate. The algebraic analog of the partial differential Schrödinger equation ($\hbar = \mu = 1$)

$$-[\Psi_{xx}(E, x, y) + \Psi_{yy}(E, x, y)]/2 + V(x, y)\Psi(E, x, y) = E\Psi(E, x, y) \quad (99)$$

is the finite-difference equation [cf (2) and (78)]:

$$-\frac{1}{2\Delta^2}[\Psi(E, n, m+1) + \Psi(E, n+1, m) - 4\Psi(E, n, m) + \Psi(E, n, m-1) + \Psi(E, n-1, m)] + V(n, m)\Psi(E, n, m) = E\Psi(E, n, m). \quad (100)$$

Suppose the required potential $V(n, m)$ is nonzero in the bounded region $G(1 < n < N;\; 1 < m < M)$:

$$V(n, m) = 0 \quad (101)$$

for $n \leqslant 1,\; n \geqslant N;\; m \leqslant 1,\; m \geqslant M$.

We determine eigenfunctions $u_\lambda(n, m)$ satisfying homogeneous conditions on the boundary S of G. For these conditions, we choose the requirement that the logarithmic derivative in the direction of the external normal to the surface at each point s on S be independent of the energy [cf (12) and (79)]:

$$\left.\begin{aligned} u(E, n, M+1) &= u(E, n, M)(1 - \Delta B_{nM}) \\ u(E, n, 0) &= u(E, n, 1)(1 + \Delta B_{n1}) \end{aligned}\right\} \text{for } n = 1, 2, \ldots, N;$$
$$\left.\begin{aligned} u(E, N+1, m) &= u(E, N, m)(1 - \Delta B_{Nm}) \\ u(E, 0, m) &= u(E, 1, m)(1 + \Delta B_{1m}) \end{aligned}\right\} \text{for } m = 1, 2, \ldots, M. \quad (102)$$

The conditions (102) make it possible to separate out from the infinite system of homogeneous algebraic equations (100) a system of $N \times M$ unknowns $u(E, n, m)$ with n and m in G. There exist $N \times M$ solutions $u_\lambda(n, m)$

$\equiv u(E_\lambda, n, m)$ for $E = E_\lambda$, $\lambda = 1, 2, \ldots, N \times M$ that form an orthonormal and complete set (the derivation is analogous to the one given in Appendix 2):

$$\sum_{n=1}^{N}\sum_{m=1}^{M} u_\lambda(n, m)\, u_{\lambda'}(n, m)\, \Delta^2 = \delta_{\lambda\lambda'}; \tag{103}$$

$$\sum_{\lambda=1}^{N\times M} u_\lambda(n, m)\, u_\lambda(n', m') = \delta_{nn'}\delta_{mm'}/\Delta^2. \tag{104}$$

Recursion Relations. We show how $V(n, m)$ can be found from E_λ and the values $u_\lambda(s)$ of the eigenfunctions on the boundary. Knowing $u_\lambda(s)$, we find from the boundary conditions (102) the functions u_λ at the points s^* that adjoin the boundary S on the outer side.

For all fixed $(n, m) = g_0$, the algebraic equation (100) relates the value of $u_\lambda(g_0)$ to u_λ at the four nearest points g_1, g_2, g_3, g_4. Thus, from (100) one can determine u_λ at the points next to S on the inner side (where $V \neq 0$) from the known values of u_λ on S and S^*, using a formula analogous to (85) [from the known values of u_λ at the four points g_1, g_2, g_3, g_0 on S and S^* we find $u_\lambda(g_4)$]:

$$u_\lambda(g_4) = 2\Delta^2 [V(g_0) - E_\lambda + 2/\Delta^2]\, u_\lambda(g_0) - u_\lambda(g_1) - u_\lambda(g_2) - u_\lambda(g_3), \tag{105}$$

bearing in mind that $V(s) = 0$.

We find the potential next to the boundary from the Schrödinger equation by means of the completeness condition (104). Multiplying Eq. (100) for $u_\lambda(g_4)$ by $u_\lambda(g_4)$ and summing over λ, we obtain with allowance for (104) [cf (17) and (86)]:

$$V(g_4) = \Delta^2 \sum_{\lambda=1}^{N\times M} E_\lambda u_\lambda^2(g_4) - 2/\Delta^2, \tag{106}$$

where $u_\lambda(g_4)$ are determined from (105).

Using the recursion relations (105) and (106), we successively find $V(g)$ and $u_\lambda(g)$ in the complete region G from the given E_λ and $u_\lambda(s)$.

Connection between E_λ and $u_\lambda(s)$. The considered example enables us to show readily that to solve the inverse problem it is sufficient to specify the values of $u_\lambda(s)$ on only part of the boundary S. Thus, in the case of a rectangular region G it is necessary to know u_λ on one of the four sides. Indeed, from these $u_\lambda(s)$ and (102) we can determine $u_\lambda(s^*)$ on a line parallel to the chosen side. In accordance with (105), from u_λ on two parallel segments of S^* and S we find u_λ on the neighboring interval of the next following line, within G. It is only to determine u_λ at the two extreme points of the segment (on S) that (102) must also be used. By means of the second recursion relation (106), we then calculate the corresponding values of V. Continuing this procedure, we find u_λ and V in the entire region G, including the boundary S.

It is remarkable that, given E_λ and $u_\lambda(s)$ on one of the sides of S, one can determine $u_\lambda(s)$ on the whole of the remaining part of the boundary.[13)]

Two-Dimensional Inverse Problem in Finite-Difference R-Matrix Theory (Method of Orthogonalization of Polynomials). The partial difference equation (100) has some features in common with the system of one-dimensional many-channel equations (78) if one of the variables, for example, m, is regarded as the channel index, and the other, n, as the only coordinate. It is true, though, that, in contrast to (78), the channels in (100) are coupled, not by means of the interaction, but through the kinetic energy operator.

We introduce auxiliary solutions φ of Eq. (100) and corresponding solutions $\mathring{\varphi}$ of the free ($V(n, m) \equiv 0$) Schrödinger equation, specifying the boundary conditions [cf (92)]:

$$\left.\begin{aligned} &\varphi_s(E, 1, m) = \mathring{\varphi}_s(E, 1, m) = \delta_{ms};\\ &[\varphi_s(E, 0, m) - \varphi_s(E, 1, m)] = \Delta\varphi_s(E, 1, m)\, B_s;\\ &[\mathring{\varphi}_s(E, 0, m) - \mathring{\varphi}_s(E, 1, m)] = \mathring{\varphi}_s(E, 1, m)\, \Delta B_s, \end{aligned}\right\} \tag{107}$$

where s is a point on $(1, m)$.

We shall assume that the lines $n = 0, 1$, where φ and $\mathring{\varphi}$ are specified, lie next to (and on the left of) the region G in which the potential $V(n, m)$ is nonzero.

Polynomial Dependence of φ and $\mathring{\varphi}$ on E. In accordance with the conditions (107), the functions φ_s and $\mathring{\varphi}_s$ are zero on the lines $n = 0, 1$, except for the points with $m = s$ on the lines $n = 1, 0$. From these values, one can, solving the corresponding partial difference equations, find φ_s and $\mathring{\varphi}_s$ at all the other sites of the coordinate mesh, nonzero values of φ_s and $\mathring{\varphi}_s$ occurring (Fig. 1) at the points within the cone with apex at $(0, s)$. At each fixed site (m, n), the functions $\varphi_s(E, n, m)$ and $\mathring{\varphi}_s(E, n, m)$ are polynomials in E of degree $n - |s - m|$. Using arguments similar to those of Berezanskiĭ,[20] we construct the polynomials $\varphi_s(E, n, m)$ as linear combinations of the known polynomials $\mathring{\varphi}(E, n', m')$:

$$\varphi_s(E, n, m) = \sum_{n'=1}^{n}\sum_{m'=m-n+n'}^{m+n-n'} \Delta^2 K(n, m; n', m')\, \mathring{\varphi}_s(E, n', m'). \tag{108}$$

For $s = m$, the coefficients of the highest powers of E in

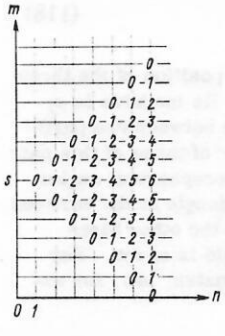

FIG. 1. Region of nonzero values of $\varphi_s(E, n, m)$, which are polynomials in E; the numbers at the sites of the mesh are the degrees of these polynomials.[20]

[13)] In addition, one can write down nonlinear connections of the type (19):

$$-1/2\Delta^4 = \sum_\lambda E_\lambda u_\lambda(n, m)\, u_\lambda(n, m \pm 1);$$

$$-1/2\Delta^4 = \sum_\lambda E_\lambda u_\lambda(n, m)\, u_\lambda(n \pm 1, m);$$

$$0 = \sum_\lambda E_\lambda u_\lambda(n, m)\, u_\lambda(n', m'),$$

where

$$(n', m') \neq (n, m), \quad (n \pm 1, m), \quad (n, m \pm 1).$$

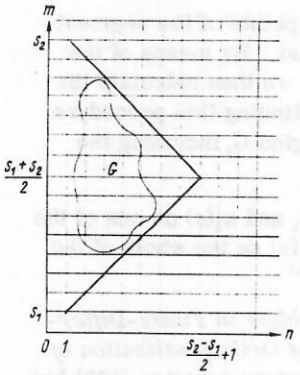

FIG. 2. At the points where $V \neq 0$ only the φ_s with s in the interval $[s_1, s_2]$ are nonzero.

$\varphi_m(E, n, m)$ do not depend on V and, therefore, are equal in $\varphi_m(E, n, m)$ and $\mathring{\varphi}(E, n, m)$; therefore $K(n, m; n, m) = 1/\Delta^2$.

To determine the remaining coefficients K in (108), we choose a complete set of functions $u_\lambda(n, m)$ such that u_λ and φ are connected by a relation of the type (93). We specify homogeneous boundary conditions for $u_\lambda(n, m)$ at mesh sites lying on the sides of the isosceles triangle with vertices $(1, s_1)$; $(1, s_2)$; $[(s_2 - s_1/2)+1, (s_2 + s_1/2)]$. The values of s_1 and s_2 must be such that the region G (Fig. 2) in which the potential is nonzero lies entirely in the triangle. Suppose that the finite-difference logarithmic derivatives of the functions u_λ and φ_s at the points $(1, s)$, $s_1 \leq s \leq s_2$, are equal:

$$[u_\lambda(0, m) - u_\lambda(1, m)] / u_\lambda(1, m) = \Delta B_s; \tag{109}$$

then as in (93) we obtain

$$u_\lambda(n, m) = \sum_{s=s_1}^{s_2} \Delta\varphi_s(E_\lambda, n, m)\, \gamma_{s\lambda}, \tag{110}$$

where

$$\gamma_{s\lambda} = u_\lambda(1, s). \tag{111}$$

Indeed, the values of any solution (100) at points $(0, s)$ and $(1, s)$ with $s_1 \leq s \leq s_2$ uniquely specify it in the complete triangle $(1, s_1)$; $(1, s_2)$; $[(s_2 - s_1/2)+1, (s_2 + s_1/2)]$, and the sum on the right-hand side of (110) is equal to u_λ at these points of the boundary and satisfies (100), since it is a linear combination of solutions φ of Eq. (100).

Gel'fand-Levitan Equations. Since $u_\lambda(n, m)$ satisfy a completeness condition of the type (104):

$$\sum_\lambda u_\lambda(n, m)\, u_\lambda(n', m') = \delta_{nn'}\delta_{mm'}/\Delta^2 \tag{112}$$

at the points (n, m) bounded by the triangle, for φ we obtain an orthogonality condition of the type (94) by substituting (110) into (112):

$$\sum_\lambda \sum_{s=m-n+1}^{m+n-1} \sum_{s'=m'-n'+1}^{m'+n'-1} \Delta^2\varphi_s(E_\lambda, n, m)\, \gamma_{s\lambda}\gamma_{s'\lambda}\, \varphi_{s'}(E_\lambda, n', m') = \delta_{nn'}\delta_{mm'}\Delta^2. \tag{113}$$

From (113) and the transformation that is the inverse of (108) it follows that $(n' < n;\ m - n + n' \leq m' \leq m + n - n')$

$$\sum_\lambda \sum_{s=m-n+1}^{m+n-1} \sum_{s'=m'-n'+1}^{m'+n'-1} \Delta^2\varphi_s(E_\lambda, n, m)\, \gamma_{s\lambda}\gamma_{s'\lambda}\, \mathring{\varphi}_{s'}(E_\lambda, n', m') = 0. \tag{114}$$

Substituting (108) into (104), we obtain the multidimensional analog of the finite-difference Gel'fand–Levitan equations [cf (96)]:

$$K(n, m; n', m') + \bar{Q}(n, m; n', m') + \sum_{n''=1}^{n-1} \sum_{m''=m-n+n''}^{m+n-n''} \Delta^2 K(n, m; n'', m'')\, \bar{Q}(n'', m''; n', m') = 0, \tag{115}$$

where $n' < n$, $m - n + n' \leq m' \leq m + n - n'$, and

$$\bar{Q}(n, m; n', m') = \sum_\lambda \sum_{ss'} \Delta^2 \mathring{\varphi}_s(E_\lambda, n, m)\, \gamma_{s\lambda}\gamma_{s'\lambda}\, \mathring{\varphi}_{s'}(E_\lambda, n', m'). \tag{116}$$

We find the connection between the potential $V(n, m)$ and K by following the procedure of the derivation of (32) and (98):

$$V(n, m) = (1/2\Delta)\{K(n, m; n-1, m) - K(n+1, m; n, m)\}. \tag{117}$$

6. FINDING THE INTERACTION IN MANY-BODY SYSTEMS

So far, we have considered different types of motion of a particle in an external field (two-body problem). Beginning with three bodies, physical systems acquire a number of qualitatively new many-particle properties. This extends the class of problems to be solved by the inverse problem theory. Thus, already in the simplest example of scattering by a target that has an internal degree of freedom, we encounter the concept of closed channels, and the question arises of the basic possibility of obtaining complete information about a system from scattering data corresponding to only the open channels. The use of inverse problem methods must help to clarify the role of many-particle forces in quantum phenomena.

From data on complex systems, it is meaningful to extract information about even the interaction of two particles (for example, information about neutron–neutron forces from neutron–deuteron experiments) if for some reason they are not available otherwise.

Hyperspherical coordinates. A particularly simple case is that of three bodies with a three-body potential that has hyperspherical symmetry, when ordinary two-body forces are absent. This means that the potential energy depends only on the modulus ρ_6 of the hyperspherical six-dimensional radius vector[14] $\rho_6 \equiv \{\rho_6, \Omega_5\}$:

$$V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = V(\rho_6) = V(\rho_6). \tag{118}$$

[14] The vector ρ_6 characterizes the relative position of the three particles in the center-of-mass system. Its modulus is $\rho_6 = \sqrt{R^2 + \rho^2}$, where ρ is the relative distance between two particles and R is the distance from the center of mass of this pair to the third particle. Among the five hyperspherical angles Ω_5, two can determine the shape of the triangle at the vertices of which the particles are situated, while the other three characterize the orientation of this triangle in space. For more details about hyperspherical coordinates, see, for example, Ref. 19.

The variables in the Schrödinger equation with this potential energy $V(\rho_6)$ separate in the hyperspherical coordinate system, i.e., the equations of motion reduce to one-dimensional differential equations for the partial hyperspherical waves:

$$\left[-\frac{1}{2}\frac{d^2}{d\rho_6^2}+\frac{\mathcal{K}(\mathcal{K}+1)}{2\rho_6^2}-E\right]F_K(\rho_6)+V(\rho_6)F_K(\rho_6)=0, \quad (119)$$

where $\mathcal{K}=K+\frac{3}{2}$; $F_K(\rho_6)$ are the coefficients of the expansion of the three-particle wave function $\Psi(\rho_6)$ with respect to the hyperspherical functions $Y_K(\Omega_5)$:

$$\Psi(\rho_6)=\sum_K F_K(\rho_6)Y_K(\Omega_5), \quad (120)$$

K is the set of five quantum numbers.

The inverse problem is formulated here in the same way as for one-dimensional motion of one particle in an external field. From the phase shift $\delta_K(E)$ of the partial hyperspherical wave and the parameters of the bound states, $V(\rho_6)$ is found (the methods set forth in Secs. 1–3 apply).

If the finite-range potential $V(\rho_6)$ does not have hyperspherical symmetry, a system of coupled equations is obtained for $F_K(\rho_6)$:

$$\left[-\frac{1}{2}\frac{d^2}{d\rho_6^2}+\frac{\mathcal{K}(\mathcal{K}+1)}{2\rho_6^2}-E\right]F_K(\rho_6)+\sum_{K'}V_{KK'}(\rho_6)F_{K'}(\rho_6)=0, \quad (121)$$

where

$$V_{KK'}(\rho_6)=\int Y_K^*(\Omega_5)V(\rho_6)Y_{K'}(\Omega_5)\,d\Omega_5. \quad (122)$$

Then in the approximation of a finite number of harmonics in (120), one can obtain from the scattering matrix $S_{KK'}(E)$ the interaction matrix $V_{KK'}(\rho_s)$, and from it determine $V(\rho_6)$ in accordance with (90).

The Problem of Closed Channels. We consider a different example of the three-body problem: scattering of a particle by a complex target consisting of a pair of particles bound by an infinite potential well $V_{12}(\rho)$. For simplicity, we restrict ourselves to the one-dimensional case.

If the functions $\Phi_\alpha(\rho)$ of the states of the pair are known, $-\Phi_\alpha''/2+V(\rho)\Phi_\alpha=\varepsilon_\alpha\Phi_\alpha$, one can expand the wave function $\Psi(R,\rho)$ of the system with respect to the complete set $\{\Phi_\alpha(\rho)\}$:

$$\Psi(R,\rho)=\sum_\alpha F_\alpha(R)\Phi_\alpha(\rho). \quad (123)$$

The coefficients $F_\alpha(R)$, the functions of the channels α, describe the motion of the particle in the field of the target in state α. They satisfy the system of coupled one-dimensional equations (see, for example, Ref. 19):

$$-F_\alpha''(R)/2+\sum_{\alpha'}V_{\alpha\alpha'}(R)F_{\alpha'}=(E-\varepsilon_\alpha)F_\alpha, \quad (124)$$

where

$$V_{\alpha\alpha'}(R)=\int\Phi_\alpha(\rho)(V_{13}+V_{23}+V_{123}(R,\rho))\Phi_{\alpha'}(\rho)\,d\rho; \quad (125)$$

$(E-\varepsilon_\alpha)$ is the energy of the particle in channel α, equal to the difference between the total energy E of the system and the target energy ε_α.

In contrast to the system of many-channel equations (78), in (124) one can have not only *open channels* ($E-\varepsilon_\alpha>0$) but also *closed channels* ($E-\varepsilon_\alpha<0$).

Let us consider the matrix of the solutions $\|F_{\alpha\beta}\|$ of the system (124), which outside the interaction region has the form [suppose $V_{\alpha\alpha'}(R\geq a)=0$]

$$F_{\alpha\beta}(E,R>a)=\delta_{\alpha\beta}\exp[-i\sqrt{2(E-\varepsilon_\alpha)}R]-S_{\alpha\beta}(E)\exp[i\sqrt{2(E-\varepsilon_\alpha)}R], \quad (126)$$

where the subscript β indicates the channel in which the incident wave is (in closed channels, $\exp[\sqrt{2(\varepsilon_\alpha-E)}R]$ plays the role of the incident wave).

To find $V_{\alpha\alpha'}(R)$, we must, for example, in the many-channel variant of Marchenko's method, specify the entire (!) scattering matrix. If the matrix elements $S_{\alpha\beta}(E)$ corresponding to open channels α and β are assumed known from a phase-shift analysis of the experimental data, the problem arises of determining the remaining part of S. Thus, for the energies E at which channel β is closed, the solutions $F_{\alpha\beta}(R)$ do not correspond to any physical process at all.

We show that in the model case of the finite-difference analog of the system of equations (124) with a bounded number of channels M there is sufficient information on the open submatrix $S(E)$ to find the complete $S(E)$. The matrices of the Jost solutions $\varphi_\pm(E,n)$, which for $n\geq N$ have the form

$$\varphi_{\alpha\beta\pm}(E,n)=\delta_{\alpha\beta}z_\alpha^{\pm n}, \quad (127)$$

where

$$z_\alpha=1-(E-\varepsilon_\alpha)\Delta^2-\sqrt{(E-\varepsilon_\alpha)^2\Delta^4-2(E-\varepsilon_\alpha)\Delta^2},$$

are polynomials in powers of the diagonal matrix $\|\delta_{\alpha\beta}z_\alpha\|^{\pm1}$ with matrix coefficients [cf (52)]:

$$\varphi_{\alpha\beta\pm}(E,n)=\delta_{\alpha\beta}z_\alpha^{\pm n}+\sum_{n'=n+1}^{N}\Delta K_{\alpha\beta}(n,n')z_\beta^{n'}. \quad (128)$$

Therefore, for the finite-difference analog of the matrix solutions (126), remembering that $F_{\alpha\beta}(E,0)=0$, we have

$$F_{\alpha\beta}(E,0)=\delta_{\alpha\beta}-S_{\alpha\beta}+\sum_{n=1}^{2N-n-3}\Delta K_{\alpha\beta}(0,n)z_\beta^{-n}-\sum_{n=1}^{2N-n-3}\Delta\sum_\delta K_{\alpha\delta}(0,n)z_\delta^n S_{\delta\beta}(E)=0. \quad (129)$$

From the M^2 algebraic equations (129), we can express $S_{\alpha\beta}$:

$$S_{\alpha\beta}(E)=\{\|\sum_{n=1}^{2N-n-3}\Delta\|K(0,n)\|\|z^n\|+I\|^{-1}\times\|I+\sum_{n=1}^{2N-n-3}\Delta\|K(0,n)\|\|z^{-n}\|\|\}_{\alpha\beta}, \quad (130)$$

i.e., the analytic form of the energy dependence of S is known to within a finite number of constant coefficients.

Since $S_{\alpha\beta}(E)$ are known for $E > \varepsilon_\alpha, \varepsilon_\beta$, these coefficients can be found from (130).

These arguments can also be extended to the limiting case $\Delta \to 0$. Then an integral equation is obtained instead of (129).

7. BRIEF ADDITIONAL COMMENTS ON INDIVIDUAL STUDIES OF THE INVERSE PROBLEM

Review Literature. The monograph Ref. 8 contains a detailed exposition of the many-channel formalism of Marchenko's method. In the book Ref. 10, in Ch. 20, a description is given of the method of the single-channel inverse problem in the Gel'fand–Levitan approach and the method of finding a spherically symmetric potential from given phase shifts $\delta_l (l = 0, 1, \ldots, \infty)$ at fixed energy (without use of the completeness property of the solutions of the Schrödinger equation); in §9 of Ch. 5, the inverse problem method in classical mechanics is considered. In the monograph Ref. 11, the stability of the Gel'fand–Levitan and Marchenko inverse problem methods are examined.

In Faddeev's second review Ref. 3 (see Ref. 9 for the first) the main attention is devoted to the multidimensional inverse problem theory.

The review literature also includes the series of papers Ref. 12, in which the inverse problem method is set forth by means of wave operators.

The use of inverse problem methods to solve nonlinear equations is reviewed in Refs. 3 and 13.

The Inverse Problem Method in the Finite-Difference Approximation. The finding of finite-difference operators from spectral characteristics is discussed in Ch. 7 of the book Ref. 20, although in it the scattering problem is not directly considered. The method is generalized to the case of finite-difference equations with operator coefficients and to the case of two dimensions.

The methods of the multidimensional finite-difference inverse problem of scattering are set forth in Refs. 21 and 22; the R-matrix variant is published for the first time in the present review.

The finite-difference analog of Gel'fand–Levitan–Marchenko theory was proposed in Refs. 4 and 5[15] (only the single-channel case).

The single-and many-channel finite-difference R-matrix inverse problem for scattering was formulated in Ref. 6. The recursion relations given in Secs. 1, 4, and 5 for finding V were obtained in Ref. 7. We can recommend the mathematical literature, Refs. 23–25, 29, in which various questions relating to the finite-difference equations are considered: convergence and stability of methods of solution as $\Delta \to 0$ (Ref. 23); mesh method for partial-difference equations (Ref. 29); proof of completeness of eigenfunctions by means of the finite-difference approach (Ref. 24); establishment of parallels between the solution of differential and finite-difference equations (Ref. 25).

Different Types of Potentials. The determination of complex-valued potentials is considered in Refs. 26 and 27; that of interactions that depend on the energy, in Ref. 28 and of a potential $V(\hat{p}^2)$ in Ref. 15. The inverse problem method for periodic potentials is considered in Ref. 43.

There exists a class of potentials (Bargman's) for which the inverse problem can be solved analytically[10] (the generalization to the many-channel case is given in Ref. 30).

Specific difficulties of the inverse problem connected with the Coulomb interaction are investigated in Refs. 31 and 32.

In Ref. 15 it is shown that the field of a rotating target can be determined from the scattering data (polarixation experiments). The inverse problem is solved for relativistic equations (Dirac, Klein–Gordon) in Ref. 33.

Other Approaches. The finding of spherically symmetric potentials from phase shifts at fixed energy is considered in Refs. 10 and 34. The continuous analog of Newton's method is used to solve the inverse problem in Ref. 35. In the series of investigations in Refs. 36, the quasiclassical approximation for finding V is considered.

All the derivatives $(d^n/dr^n)V(r)$ at $r = 0$ can be calculated by the method proposed in Ref. 37, which is equivalent to information about $V(r)$ in the region in which the Taylor series for $V(r)$ converges. In the case of symmetric (one-dimensional) potentials it is sufficient for the determination of V to specify only E_λ (Ref. 38) (without γ_λ) if the two-spectrum theorem[39] is used. Information about the finding of the so-called separable potentials can be found in the book Ref. 42.

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APPENDIX 1: FINITE-DIFFERENCE ANALOG OF R-MATRIX SCATTERING THEORY

The wave function $\Psi(E, n)$ for $n \geq N$, i.e., for $r \geq a$, where $V(r) = 0$ or where V is known, has the form [see (48) and (54)]:

$$\Psi(E, n \geqslant N) = A[I(E, n) - S(E)\, O(E, n)], \qquad \text{(A.1)}$$

where I and O are the known incident and scattered waves, which for the free finite-difference Schrödinger equation ($V = 0$) correspond to $\exp(\pm ikr)$ [see (49) and (49a)]:

[15] The equations of this approach differ from the corresponding equations of this review. For example, instead of the Schrödinger equation (2) the equation $[\Psi(E, n+1) + \Psi(E, n-1)]/2 = (1 - E\Delta^2)\exp[\Delta^2 V(n)]\Psi(E, n)$, is considered, and instead of Eqs. (31), (47), and (58) more complicated equations are obtained (this also applies to Ref. 6, in which the relation $K(n, n) = 1/\Delta$ was not taken into account).

$$I(E, n)=z^{-n};\ O(E, n)=z^{+n}. \tag{A. 2}$$

If the potential has a known tail for $r \geq a$, then I and O are solutions with the asymptotic behavior (A. 2) and are assumed known for $r \geq a$.

We introduce the function $\mathcal{R}(E)$, which is related to the finite-difference logarithmic derivative of $\Psi(E, n)$ at the point a:

$$[\Psi(E, N+1)-\Psi(E, N)]\ \Delta\Psi(E, N)=(a\Delta)^{-1}. \tag{A. 3}$$

We expand $\Psi(E, n)$ with respect to the complete set of functions $u_\lambda(n)$ on the interval $0<n\leq N$ [see (14)][16]:

$$\Psi(E, n)=\sum_{\lambda=1}^{N} A_\lambda(E)\, u_\lambda(n), \tag{A. 4}$$

where $A_\lambda(E)$ have, on the basis of (14), the form

$$A_\lambda(E)=\sum_{n=1}^{N} \Psi(E, n)\, u_\lambda(n)\, \Delta \tag{A. 5}$$

We multiply (2) by $u_\lambda(n)$, the equation for $u_\lambda(n)$ by $\Psi(E, n)$, subtract the second from the first, sum the result over n, and, using (A. 5), we obtain

$$A_\lambda(E)\,(E-E_\lambda)=\{-\Psi(E, N+1)\, u_\lambda(N)+\Psi(N)\, u_\lambda(N+1)\}\, 2\Delta. \tag{A. 6}$$

We add and subtract $\Psi(E, N)u_\lambda(N)$ in the curly brackets of (A. 6) and substitute $A_\lambda(E)$ from (A. 5) into (A. 3):

$$\Psi(E, n)=\frac{1}{2}\sum_{\lambda=1}^{N}\frac{u_\lambda(n)}{E-E_\lambda}\left\{\Psi(E, N)\,\frac{u_\lambda(N+1)-u_\lambda(N)}{\Delta}-u_\lambda(N)\times\frac{\Psi(E, N+1)-\Psi(E, N)}{\Delta}\right\}. \tag{A. 7}$$

Taking into account (A. 3) and (12), we obtain

$$R(E)\equiv\mathcal{R}(E)/[1-\mathcal{R}(E)\, B]=\sum_{\lambda=1}^{N}[\gamma_\lambda^2/(E_\lambda-E)], \tag{A. 8}$$

where E_λ and γ_λ^2 determine the positions of the resonances of the R-matrix and their reduced widths.

The connection between $R(E)$ and the scattering matrix can be established in accordance with (A. 1), (A. 3), and (A. 8):

$$R(E)=\sum_\lambda\frac{\gamma_\lambda^2}{E_\lambda-E}=\frac{\Delta}{a}\,\frac{I(N)-S(E)\,O(N)}{I(N+1)-I(N)-S(E)\,[O(N+1)-O(N)]-(B\Delta/a)\,I(N)+(B\Delta/a)\,S(E)\,O(N).} \tag{A. 9}$$

Thus, the zeros of the known expression in the denominator of the fraction on the right-hand side of (A. 9) determine the values $E=E_\lambda$ and the corresponding γ_λ can be found in accordance with (A. 8):

$$\gamma_\lambda^2=\lim_{E\to E_\lambda}\{R(E)\,(E-E_\lambda)\}, \tag{A. 10}$$

using (A. 9) and l'Hôpital's rule for calculating the limit (of the type 0/0).

If the required potential contains bound states with energy ε_i, then, taking the constant B equal to $a\sqrt{2\varepsilon_1}$, one can take the ground level $-\mathcal{R}_1$ coincident with E_1. The remaining parameters $E_\lambda<0$ can be determined by means of the relations

$$(\sqrt{2\varepsilon_1}-\sqrt{2\varepsilon_i})^{-1}=a\sum_{\lambda}^{N}[\gamma_\lambda^2/(\varepsilon_i-E_\lambda)]. \tag{A. 11}$$

In the case of M coupled channels, we obtain instead of (A. 3)[44]

$$F_\alpha(E, N)=\sum_{\alpha'=1}^{M}R_{\alpha\alpha'}\{[F_{\alpha'}(E, N+1)-F_{\alpha'}(E, N)]\,a/\Delta-B_{\alpha'}F_{\alpha'}(E, N)\}. \tag{A. 12}$$

Using the condition of completeness (81) of the solutions $u_{\alpha\lambda}(n)$, we can, as in (A. 4)–(A. 8) obtain

$$R_{\alpha\alpha'}(E)=\sum_{\lambda=1}^{N\times M}[\gamma_{\alpha\lambda}\gamma_{\alpha'\lambda}/(E_\lambda-E)]. \tag{A. 13}$$

We find the connection between $R_{\alpha\alpha'}$ and the scattering matrix S by substituting the asymptotic behavior of the matrix of solutions (78) into (A. 12).

APPENDIX 2: CONDITIONS OF COMPLETENESS OF THE SOLUTIONS OF THE SCHRÖDINGER EQUATION

Equation (2) is a special case of the many-channel system (78), and we shall therefore only derive the completeness relation for the eigenfunctions $u_{\alpha\lambda}(n)$.

We multiply Eq. (78) for $u_{\alpha\lambda}(n)$ by $\Delta u_{\alpha\lambda'}(n)$ and the equation for $u_{\alpha\lambda'}(n)$ by $\Delta u_{\alpha\lambda}(n)$, subtract the one equation from the other, and sum over the channel index α from 1 to M. The terms containing the elements of the interaction matrix $V_{\alpha\alpha'}(n)$ then vanish because of its symmetry $V_{\alpha\alpha'}(n)=V_{\alpha'\alpha}(n)$. Summing both sides of the resulting equation over n from 1 to N, reducing like terms, and taking into account the boundary conditions (79), we obtain

$$(E_\lambda-E_{\lambda'})\sum_{\alpha=1}^{M}\sum_{n=1}^{N}\Delta u_{\alpha\lambda}(n)\, u_{\alpha\lambda'}(n)=0. \tag{A. 14}$$

Therefore, for $\lambda\neq\lambda'$ the eigenvectors are orthogonal and they can be normalized to unity. As a result, we obtain

$$\sum_{\alpha=1}^{M}\sum_{n=1}^{N}\Delta u_{\alpha\lambda}(n)\, u_{\alpha\lambda'}(n)=\delta_{\lambda\lambda'}. \tag{A. 15}$$

We obtain the completeness condition for $u_{\alpha\lambda}$ by multiplying both sides of (A. 15) by $u_{\alpha'\lambda'}(m)$, summing over λ', and reversing the order of integration:

[16] The expansion (A. 4) does not hold at the point $n=N+1$ since this point is outside the interval $0<n\leq N$, where $u_\lambda(n)$ form a complete set. Therefore, to (A. 4) one cannot apply right finite-difference differentiation (see footnote 10) at the point $n=N$. This explains the fact that in ordinary B-matrix theory (when r is a continuous coordinate) the expansion $\Psi(E, r)=\sum_\lambda A_\lambda(E)u_\lambda(n)$ converges at $r=a$ nonuniformly and cannot be differentiated there.

$$\sum_{\alpha=1}^{M}\sum_{n=1}^{N}\{\Delta\sum_{\lambda=1}^{N}u_{\alpha'\lambda'}(m)\,u_{\alpha\lambda}(n)\}\,u_{\alpha\lambda}(n)=u_{\alpha'\lambda'}(m). \tag{A.16}$$

Indeed, the expression in the curly brackets on the left-hand side in (A. 16) acts like $\delta_{mn}\delta_{\alpha\alpha'}$, i. e., we have the Parseval equation (81):

$$\sum_{\lambda=1}^{N}u_{\alpha'\lambda}(m)\,u_{\alpha\lambda}(n)=\delta_{mn}\delta_{\alpha\alpha'}/\Delta. \tag{A.17}$$

The conditions of orthogonality (A. 15) and completeness (A. 17) can be cast into a more symmetric form by combining the solutions u for different energies into matrices $\hat{u}$ of dimension $(N\times N)$ in the single-channel case and $(N\cdot M\times N\cdot M)$ in the M-channel case:

$$\hat{u}^{+}\hat{u}=\hat{1};\quad \hat{u}\hat{u}^{+}=\hat{1}. \tag{A.18}$$

Here, $\hat{1}$ are unit matrices. In the case of one channel, λ and n serve as conjugate indices of the matrix elements; for many channels, λ and the double index αn play this role.

APPENDIX 3: DERIVATION OF THE CONNECTION BETWEEN $V(n)$ AND $K(m,n)$

We shall proceed as in the case of a continuous coordinate (see Ref. 41, p. 410). We substitute φ_{+} in the form (53) into the finite-difference Schrödinger equation (2), (52). We use (10) and (20a) to cancel some of the terms in the resulting equation and express $E\varphi_{+}(n)$ in terms of $\mathring{\varphi}_{+}(n)$, $\mathring{\varphi}_{+}(n\pm1)$. After simple transformations, taking into account $\mathring{\varphi}_{+}(n)=\exp(i\theta n)$, we obtain

$$\sum_{m=n-1}^{N}\Delta A(m)\exp(i\theta m)+B\exp(i\theta n)+C=0, \tag{A.19}$$

where

$$A(m)=-[K(n-1,m)-2K(n,m)+K(n+1,m)]/2\Delta^{2}$$
$$-[K(n,m-1)-2K(n,m)+K(n,m+1)]\,2\Delta^{2}+V(n)\,K(n,m); \tag{A.20}$$
$$B=-[K(n-1,n)-K(n,n+1)]\,2\Delta+V(n); \tag{A.21}$$
$$C=K(n,N+1)\exp(i\theta N\,2\Delta)-K(n,N)\exp[i\theta(N+1)]/2\Delta. \tag{A.22}$$

Since (A. 19) is satisfied for all θ, the coefficients of $\exp(i\theta m)$ with different values of m must vanish, i. e.,

$$A(m)=0;\quad C=0;\quad B=0. \tag{A.23}$$

From the first and the second equation in (A. 23), we obtain a partial difference equation and one boundary condition for $K(n, m)$:

$$[K(n+1,m)-2K(n,m)+K(n-1,m)]\,2\Delta^{2}+V(n)\,K(n,m)$$
$$-[K(n,m+1)-2K(n,m)+K(n,m-1)]\,2\Delta^{2}=0; \tag{A.24}$$
$$[K(n,N+1)-K(n,N)]/K(n,N)$$
$$=[\mathring{q}_{+}(E,N+1)-\mathring{q}_{+}(E,N)]\,\mathring{q}_{-}(E,N). \tag{A.25}$$

From the third equation in (A. 23), we obtain expression (60):

$$V(n)=[K(n,n+1)-K(n-1,n)]/2\Delta. \tag{A.26}$$

In the many-channel case, the matrix generalizations of (A. 19)–(A. 26) are obtained similarly.

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