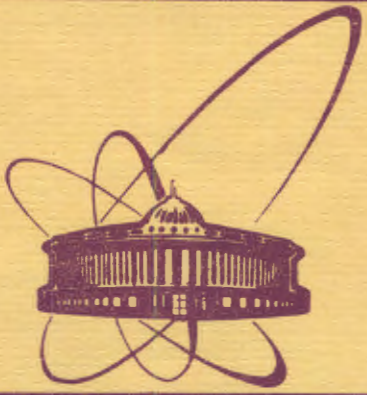

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Submitted to "Известия АН СССР" /сер. физ./

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Уравнение Шредингера-Штермера в прямой и обратной задачах рассеяния

Показано, как следует задавать граничные условия для уравнения Шредингера-Штермера (Ш-Ш), не прибегая к стартовым методам, что принципиально важно для решения соответствующей конечно-разностной обратной задачи. Аналогичный рецепт годится и для других разностных аппроксимаций высших порядков для уравнения Шредингера, а также в методе конечных элементов с нелинейными сплайнами. Предложено обобщение R -матричной теории рассеяния для уравнения Ш-Ш. Получены рекуррентные соотношения, с помощью которых решается ОЗ для уравнения Ш-Ш.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1979

Melnikov V.N., Suzko A.A., Zakhariev B.N. **E4 - 12251**

Schroedinger-Stermer Equation in Direct and Inverse Scattering Problems

It is shown how to formulate boundary conditions for the Scroedinger-Stermer (S-S) equation without using starting methods, what is of principle significance for the solution of a relevant finite-difference (f-d) inverse problem. The same rule is valid for other higher order f-d approximation for the Schroedinger equation and for finite element methods with nonlinear splines. A generalization for R -matrix scattering theory for S-S equation is suggested. The recurrence relations, which give the solution of inverse problem for S-S equation are derived.

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

Preprint of the Joint Institute for Nuclear Research. Dubna 1979

For practical solutions of quantum mechanical problems finite-difference (f-d) analogues of the Schroedinger equation are widely used. The simplest discretization scheme is the Euler method in which instead of second order differential equation

$$-\Psi''(r) + V(r)\Psi(r) = E\Psi(r) \qquad (1)$$

just the second order f-d equation

$$-\frac{1}{\Delta^2}\{\Psi(n-1) - 2\Psi(n) + \Psi(n+1)\} + V(n)\Psi(n) = E\Psi(n) \qquad (2)$$

is considered. The accuracy of approximation of (1) by (2) does not exceed $\sim\Delta^2$ (Δ - is a f-d step).

More perfect is the Stermer scheme /1/, in which eq. (1) is approximated by 4th order (or more higher order) f-d equation:

$$-\frac{4}{\Delta^2}\{\Psi(n-2) - \Psi n-1) - \Psi(n+1) + \Psi(n+2)\} + 5V(n-1)\Psi(n-1) + \qquad (3)$$

$$+2V(n)\Psi(n) + 5V(n+1)\Psi(n+1) = E[\,5\Psi(n-1) + 2\Psi(n) + 5\Psi(n+1)\,].$$

The accuracy of eq. (3) is $\sim\Delta^4$. Further we will consider special questions of using Schroedinger-Stermer (S-S) eq. (3) in direct and inverse problems. It will be shown , how to formulate additional "boundary" conditions

in order to avoid "unphysical" waves, which exist in general solutions due to the fact that the order of eq. (3) is by two units higher than that of eq. (2) and eq. (1)*. It appears that these new boundary conditions allow one to determine Ψ in four initial points (what we need, to begin numerical solution of eq. (3)) without using starting methods /2/. The generalized orthonormalization and completeness conditions for eigenstates of S-S equation (3) with homogeneous boundary conditions will be given, and the corresponding R-matrix scattering theory will be formulated.

We shall show how to reconstruct the potential $V(n)$ in (3) from the scattering data (spectral parameters) using the recurrence relations which generalize those for Euler scheme /3,4/. Thus we get a solution of f-d inverse problem model for Stermer scheme.

But in order to get an algorithm of approximate reconstruction of the potential $V(r)$ in (1) on the basis of this model, we need also to find a transformation rule $S_S \to S_{S-S}$, where S_{S-S} are the spectral data for S-S inverse problem, and S_S are the corresponding values for eq. (1). This problem is not yet solved (for Euler scheme this is done in /5/).

DIRECT PROBLEM, "BOUNDARY" CONDITIONS

For a unique choice of solution for S-S eq. (3), we need four "boundary" conditions,

* We use the term "boundary" conditions for f-d equations by analogy with the differential equations.

because eq. (3) is of fourth order (instead of two conditions for eqs. (1) and (2)). Two conditions of these four will be chosen as for the Schroedinger eq. (1) or its f-d analog (2). To make it clear what additional conditions we need, it is instructive to consider the general solution of eq. (3) in the region where $V(n)=0$ (free motion of waves) and S-S equation has constant coefficients.

A standart form of a particular solution for such an equation is z^n. Insertion of z^n in S-S equation with $V=0$ gives for z an algebraic equation (of fourth degree):

$$z^4+z^3(5\frac{\Delta^2 E}{4}-1)+z^2\frac{\Delta^2 E}{2}+z(\frac{5\Delta^2 E}{4}-1)+1=0. \qquad (4)$$

This equation has four roots:

$$z_{1,2}=\frac{1}{z_{3,4}}=\cos\theta_{1,2}+i\sin\theta_{1,2}=e^{\pm i\theta_{1,2}}, \qquad (5)$$

where

$$4\cos\theta_{1,2}=1-\frac{5\Delta^2 E}{4}\pm\sqrt{(1-\frac{5\Delta^2 E}{4})^2-2\Delta^2 E+8}. \qquad (6)$$

So the general solution of S-S equation with $V=0$ is a linear combination of four waves:

$$\Psi(n)=A e^{i\theta_1 n}+Be^{-i\theta_1 n}+Ce^{i\theta_2 n}+De^{-i\theta_2 n}. \qquad (7)$$

For small values of energy ($\Delta^2 E \ll 1$) $\theta_1 \sim \Delta\sqrt{E}$, i.e., θ/Δ corresponds to the wave number of initial Schroedinger eq. (1). Therefore we shall call $e^{\pm i\theta_1 n}$ the "physical" waves and $e^{\pm i\theta_2 n}$ with different energy dependence of the wave number θ_2/Δ the unphysical ones. The appearance of unphysical waves is a distinctive property of solution of

S-S equation in comparison with eqs. (1), (2). It is reasonable therefore to take as the additional boundary conditions the requirements that coefficients C and D in eq. (7) be zero.

Let us write down these conditions in terms of linear combinations of Ψ values at boundary points. Taking into account eq. (7) it is easy to see that the terms with coefficient A disappear in expressions $\Psi(n)\, z_1 - \Psi(n+1)$ and $\Psi(n+1)\, z_1 - \Psi(n+2)$. And there are only the terms with C and D in expression

$$\Psi(n) - \Psi(n+1)\,(z_1 + z_1^{-1}) + \Psi(n+2), \qquad (8)$$

i.e., there are only unphysical waves in expression (8). So, the requirement that expression (8) be zero for two different values of n is equivalent to the conditions that coefficients C and D in (7) are zero (because two homogeneous linear independent combinations of C and D are zero).

Let us consider now the case of wave penetration through the bounded region ($a \leq r \leq b$), with nonzero potential. Following the logic of the preceding discussion we need in addition to two physical conditions (for example, a certain, normalization of the physical wave approaching the interaction region from the left and the absence of the physical wave going to the potential zone from the right) that unphysical waves ($e^{\pm i\theta_2 n}$) disappear from both sides of potential obstacle. In all this means six boundary conditions, what is more than we can require for an equation of fourth order.

Fortunately it appears that it is enough to destroy the unphysical waves from one side of the interaction region only. Then the unphysical waves will have very small amplitudes ($\sim\Delta^4$, so that they can be neglected) also from the other side. This is due to uniqueness of solution of eq. (3) with four boundary conditions and to the special construction of eq. (3) that its proper solution does not deviate from the one of eq. (1) more than by $\sim\Delta^4$ *.

It is obvious that in particular (limit) case of zero potential the requirement of zero amplitude of the wave $e^{-i\theta_2 n}$ from the one side leads to its exact disappearance also from the other side (the same is true for $e^{+i\theta_2 n}$). In the general case we have to demand that the expression (8) becomes zero at two points $n = n_1$ and $n = n_2$ from any side of the potential barrier (no matter together or separately).

Up to now, in order to begin the numerical calculations according to the Stermer scheme, the values of wave function in four neighbour points were determined using another approximate scheme (i.e., Euler scheme but with such a small step $\Delta_E \ll \Delta$, that the error does not exceed Δ^4).

The suggested way to formulate the boundary conditions allows the use of the unique Stermer scheme without a cumbersome combination of different approaches.

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* This is true only for the lowest part of the energy spectrum, where Stermer approximation is practically used.

In the same way the boundary conditions can be formulated for other higher order f-d approximations to Schroedinger eq. (i.e., for S-S- equation of 6th order).

ORTHONORMALIZATION OF EIGENFUNCTIONS,

which correspond to S-S equation has its peculiarity due to the three diagonal matrix $\hat{K}(K_{ii}=2; K_{i,i\pm1}=5)$ which stands in the right-hand-side of eq. (3).

It is most simple to show the orthogonality of solutions of (3), which satisfy the homogeneous boundary conditions, without energy dependence. But in expression (8), which we use to descroy the unphysical waves, the energy dependence is introduced through z (see (5), (6)). Nevertheless, if in R-matrix formalism with potential equal to zero for $r > a = \Delta(N-1)$ we use* "physical" condition (which can be used in Euler scheme /3-5/):

$$u(0)=0; \quad u(N+1)=0, \tag{9}$$

and choose in (8) the two values $n_1=0$ and $n_2=N+1$ the energy dependence will disappear in additional boundary conditions:

$$u(-1)+u(1)=0; \quad u(N)+u(N+2)=0. \tag{10}$$

There are N solutions $u_\lambda(n)$ for discrete (finite) set of eigenstates $E=E_\lambda$ (resonance positions of R-matrix).

* Or for the potentials, for which there is an analytical solution at $r \geq a$.

It is worth noting that together with the disappearance of z_1-dependence in boundary conditions (10), we lose the indication, what waves have to be destroyed (physical or unphysical). So the complete set of eigenfunctions u_λ consists both of physical and unphysical states. Strictly speaking, instead of an ordinary orthogonality of eigenfunction, corresponding to different energy state, there is <u>biorthogonality</u> of the set $\{u_\lambda\}$ and the functions u_λ^T, corresponding to the system of algebraic equations like (3), (9), (10) but with a transponed matrix of coefficients.

Taking into account that symmetrization of this matrix leads to the changes of an order of $\sim\Delta^4$, which can be neglected, we can use instead of (3) the equation with symmetrized matrix:

$$-\frac{4}{\Delta^2}\{\Psi(n-2)-\Psi(n+1)+\Psi(n+2)\}+5\frac{V(n)+V(n-1)}{2}\Psi(n-1)+ \tag{11}$$

$$+2V(n)\Psi(n)+5\frac{V(n+1)+V(n)}{2}\Psi(n)=E[\,5\Psi(n-1)+2\Psi(n)+5\Psi(n+1)\,].$$

The orthonormalization condition is derived by multiplying by $u_{\lambda'}(n)$ eq. (11) for $u_\lambda(n)$ with $E=E_\lambda$ and eq. for $u_{\lambda'}(n)$ with $E=E_{\lambda'}$ by $u_\lambda(n)$, subtracting one of these equations from the other and summing the result over n (taking into account eqs. (9) and (10)):

$$\sum_{n,m=1}^{N} u_\lambda(n)\,K(n,m)\,u_{\lambda'}(m)=\delta_{\lambda\lambda'}/\Delta\,, \tag{12}$$

where $||K||$ is the above-mentioned three-diagonal matrix, which acts on the function in the right-hand side of eqs. (3), (11). The appearance of this weight factor K in

generalized orthonormalization (12) is one of the peculiarities of the considered Stermer scheme (in comparison with Euler method [3-5]). The completeness relation (orthonormalization over the energy variable λ) is derived from eq. (12), multiplying it by $u_\lambda(p)$ summing both sides of equation over λ and changing the order of summation:

$$\sum_{\lambda,n=1}^{N} u_\lambda(p)\, u_\lambda(n)\, K(n,m) = \delta_{pm}/\Delta. \qquad (13)$$

Another form of generalized Parceval equation is:

$$\sum_{\lambda=1}^{N} u_\lambda(m)\, u_\lambda(n) = K^{-1}(n,m). \qquad (14)$$

Now let us use eqs. (12), (13) for discrete parametrization of the scattering data.

R-MATRIX SCATTERING THEORY

The wave function Ψ, corresponding to the scattering state with asymptotic behaviour:

$$\Psi = e^{-i\theta_1 n} - S(E)\, e^{i\theta_1 n} \qquad (15)$$

can be expanded in the complete set of eigenfunctions satisfying eqs. (9)-(11)

$$\Psi(E,n) = \sum_{\lambda=1}^{N} A_\lambda(E)\, u_\lambda(n). \qquad (16)$$

According to eqs. (12) and (16), the coefficients $A_\lambda(E)$ can be written as:

$$A_\lambda(E) = \sum_{n,m=1}^{N} \Delta\, \Psi(E,n)\, K(n,m)\, u_\lambda(m). \qquad (17)$$

Multiplying eq. (11) by $u_\lambda(n)$ and eq. for $u_\lambda(n)$ by $\Psi(E,n)$ subtracting one of these

equations from the other and summing over n, we get, taking into account the boundary conditions (9), (10) for u_λ and putting that $\Psi(-1)+\Psi(1)=0$:

$$A_\lambda(E) = \frac{4}{\Delta^2}\,\frac{\Psi(N+1)}{E_\lambda - E}\,\{u_\lambda(N-1) + u_\lambda(N)[\,z_1 + z_1^{-1} - 1 - 5E\frac{\Delta^2}{4}]\} \qquad (18)$$

Substituting A_λ from (18) into (16), we get for $n=N$ and $n=N-1$

$$\Psi(N)/\Psi(N+1) = \frac{4}{\Delta}\sum_{\lambda=1}^{N}\frac{u_\lambda(N)}{E_\lambda - E}\{u_\lambda(N-1) + \qquad (19)$$

$$+ u_\lambda(N)[\,z_1 + z_1^{-1} - 1 - 5E\,\frac{\Delta^2}{4}]\}$$

$$\Psi(N-1)/\Psi(N+1) = \frac{4}{\Delta}\sum_{\lambda=1}^{N}\frac{u_\lambda(N-1)}{E_\lambda - E}\{u_\lambda(N-1) + \qquad (20)$$

$$+ u_\lambda(N)[\,z_1 + z_1^{-1} - 1 - 5E\frac{\Delta^2}{4}]\}\,.$$

The left-hand side of eqs. (19), (20) can be determined due to eq. (15) if we know the scattering matrix. So, the S(E) is parametrized by the set of 3N values $\{E_\lambda, u_\lambda(N), u_\lambda(N-1)\}$. If S(E) is known, these parameters can be determined from eqs. (19), (20). In particular the zeroes of $\Psi(E,N+1)$ give E_λ. The functions are determined up to the sign, which is not significant from the physical point of view. So eqs. (19), (20) are the extension of the results of the R-matrix theory for S-S equation.

INVERSE PROBLEM

After the determination of values $u_\lambda(N)$, $u_\lambda(N-1)$ from eqs. (19) and (20), the second

equations in (9) and (10) give us the values $u_\lambda(N+1)$ and $u_\lambda(N+2)$. Starting from these known values of eigenfunctions in four neighbour points, we can determine $u_\lambda(n)$ and $V(n)$ in the whole interaction region. Let $V(n \geq N) = 0$. Then $u_\lambda(N-2)$ can be expressed from eq. (11) through the known values of eigenfunctions:

$$u_\lambda(N-2) = u_\lambda(N-1) + u_\lambda(N+1) - u_\lambda(N+2) + [\,5\frac{V(N)+V(N+1)}{2} u_\lambda(N+1) +$$

$$+2V(N)\,u_\lambda(N) + 5\frac{V(N-1)+V(N)}{2} u_\lambda(N-1)\,] + \frac{\Delta^2 E}{4}[\,5u_\lambda(N+1) + \quad (21)$$

$$+2u_\lambda(N) + 5\,u_\lambda(N-1)\,].$$

The expression for $V(N-1)$ is derived after multiplication of eq. (11) with $n = N$ by $\sum_m K(N-1,m)\,u_\lambda(m)$ and summation over λ (the orthonormalization conditions (13), (14) - completeness relations should be also taken into account):

$$V(N-1) = \sum_{\lambda,m,p=1} K(N,m)\,u_\lambda(m)\,E_\lambda\,K(N-1,p)\,u_\lambda(p) - \frac{4}{\Delta^2} \qquad (22)$$

The system of eqs. (21), (22) allows one to make a first step inside the interaction region while solving the inverse scattering problem. Repeating analogous operations we find $u_\lambda(n)$ and $V(n)$ at the next points, using the recurrence relations of the type (21), (22), successively.

The authors are grateful to I.V.Amirkhanov, J.Bang, E.B.Plekhanov, B.V.Rudjak for discussions concerning the subject of this paper.

APPENDIX

Infinitely Deep Potential Well

Let $V(n) = V_0$ at $0 < n < N+1$ and $V(0) = V(N+1) = \infty$. Eq. (11) with boundary conditions (9), (10) has solutions $u_\lambda(n) = A\sin\theta_\lambda n$ with $\theta_\lambda = \frac{\lambda\pi}{N+1}$. The corresponding energy levels E_λ are determined from the following equation (see eq. (6)):

$$4\cos\frac{\lambda\pi}{N+1} = 1 - \frac{5\Delta^2 E_\lambda}{4} + \sqrt{(1 - \frac{5\Delta^2 E_\lambda}{4})^2 - 2\Delta^2 E_\lambda + 8}\,.$$

For small values λ and $\Delta^2 E$, we get (choosing + sign):

$$E_\lambda = (\frac{\pi\lambda}{\Delta(N+1)})^2 + o(\Delta^4).$$

So the lowest, "physical" energy levels in infinitely deep rectangular potential well, derived from S-S equation coincide (within the accuracy $\sim\Delta^4$) with the corresponding values for Schroedinger equation.

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Received by Publishing Department
on February 13 1979.