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A Newtonian iteration scheme with the Schwinger variational functional for solving a scattering problem

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Abstract: A Newtonian iteration scheme has been constructed for solving a scattering problem using the Schwinger variational functional. The scattering problem is formulated as an eigenvalue problem with respect to a pair of unknown variables: a phase shift and a wavefunction. The efficiency and accuracy of the proposed iteration scheme are demonstrated on exact solvable tasks of an elastic scattering problem with Morse and spherical well potentials.

Keywords: Elastic scattering; variational methods; phase shift; integral equations; Newtonian methods.

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1 Introduction

In nuclear physics, scattering problems are connected to calculations of the scattering amplitude, phase shifts and mixing parameters, comprising the definition of the asymptotic wavefunctions of Schrödinger equation with a short-range potential $\mathbf{V}$. To solve a scattering problem, different methods are used. One of the wide-spread approaches is the Schwinger variational method. The method uses the following expression for the variational functional:

$$f(\mathbf{k},\mathbf{k}') = -\frac{\mathbf{1}}{\mathbf{2}\pi}\frac{(\mathbf{k}'|\mathbf{V}|\eta_{\mathbf{k}}^{(+)})(\eta_{\mathbf{k}'}^{(-)}|\mathbf{V}|\mathbf{k})}{(\eta_{\mathbf{k}'}^{(-)}|\mathbf{V}-\mathbf{V}\mathbf{G_0}\mathbf{V}|\eta_{\mathbf{k}}^{(+)})}, \tag{1}$$

which allows one to calculate amplitudes and scattering phases more accurately than in Born?s approximation [1, 2]. Here $|\eta)$ are basis functions, G_0 is a Green's free function. As shown in [3, 4], it is possible to find effectively arbitrary solutions of a scattering problem by means of different

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iteration schemes constructed on the basis of the Schwinger variational functional Eq (1), using a separable approximation for a short-range potential

$$\left\{ \begin{array}{l} V^{(N)} = \sum_{i,j=1}^{N} V|\eta_i) d_{ij}^{(N)} (\eta_j|V; \\ d_{ij}^{-1} = (\eta_i|V|\eta_j), \end{array} \right. . \tag{2}$$

Nevertheless, the problems of constructing the stable iteration schemes permitting to calculate solutions with a predetermined accuracy, require urgent solutiuon.

In paper [5], a stable iteration scheme has been constructed for solving the scattering problem for Schrödinger equation, on the basis of the Continuous Analogue of Newton's Method (CANM), and using the additional Hulthen variational functional. In this paper, the CAMN is applied to solve a scattering problem with a given accuracy, in the framework of the integral equation and using the additional Schwinger variational functional Eq (1).

This paper is composed as follows. The second section deals with a general consideration required for constructing the stable iteration schemes for solving spectral problems on the basis of CANM. The possibility of constructing various known iteration schemes for spectral problems on the basis of CANM has been discussed.

In the third section, using a variational Schwinger functional, the scattering problem is formulated as an eigenvalue problem with respect to a pair of unknown variables: a phase shift and a wavefunction. A stable iteration scheme is constructed on the basis of CANM and its modifications in the vicinity of the solution under consideration.

The fourth section demonstrates the efficiency of the proposed iterative scheme and its accuracy on exact solvable tasks of the elastic scattering problem with a Morse potential and a spherical well potential.

2 The Continuous Analogue of Newton's Method

Let us consider a scheme of solving spectral problems on the basis of the Continuous Analogue of Newton's Method which consists of substitution of a source nonlinear stationary problem

$$\varphi(a, \lambda, y) = 0 \tag{3}$$

with respect of unknowns $z = (\lambda, y) \in R^n \times Y$, $Y \subseteq B$ at a fixed set of the physical vector parameter $a \in R^m$ by the evolutionary Cauchy problem [6]

$$\varphi'(a, z(t)) \frac{dz(t)}{dt} = -\varphi(a, z(t)), \tag{4}$$

$$z(0) = z_0. \tag{5}$$

Here t $(0 \le t < \infty)$ is a continuous parameter that depends on trajectory $z(t)$, φ' is the Frechet derivative , z_0 is the element in the vicinity of the required solution $z^* = (\lambda^*, y^*)$ to Eq (3). The proof of the convergence of the continuous trajectory $z(t)$ at $t \to \infty$ to solution z^* under the conditions of continuity φ , φ' and existence of the restricted operator $(\varphi')^{-1}$ in the vicinity z^* is based on the integral of the Cauchy problem Eq (4) - Eq (5)

$$\varphi(a, z(t)) = e^{-t} \varphi(a, z_0). \tag{6}$$

The discrete approximation over argument t of the problem Eq (4) - Eq (5) on the basis of the Eulerian representation reduces it to solving a succession of linear problems

$$\begin{array}{l} \varphi'(a, z_k) \Delta z_k = -\varphi(a, z_k), \\ z_{k+1} = z_k + \tau_k \Delta z_k, \end{array} \tag{7}$$

and a special choice of parameter τ_k can optimize the rate and stability of convergence $z_k \to z^*$ [7, 8]. For the classical spectral problems with respect to pair $z = \{\lambda,\ \Psi\} \in R^n \times Y$, the nonlinear equation Eq (3) can be represented in the form

$$\varphi(a, \lambda, \Psi) = \begin{pmatrix} (H(a) - \lambda I)\Psi \\ F(a, \lambda, \Psi) \end{pmatrix} = 0. \tag{8}$$

Here $H(a)$ is the operator in the Hilbert space, and $F(a, \lambda, \Psi)$ is an additional functional, for example,

$$\begin{array}{ll} \text{a). } (\Psi, \Psi) - 1 = 0 & \text{a normalization condition} \\ \text{b). } (\Psi, (H(a) - \lambda I)\Psi) = 0 & \text{an orthogonality condition.} \end{array} \tag{9}$$

To solve the spectral problems Eq (8), the iteration scheme Eq (7) is applicable. A two-component structure of function φ and the possibility of varying functional F in iterations allow one to receive a wide set of iteration processes with adjustable properties, including the known methods of inverse iterations, inverse iterations with the Rayleigh shift, etc.

The iteration scheme Eq (7) for Eq (8) at a fixed value of the vector parameter a represents at each step of iterations a system with respect to the iterative correction $\Delta z_k = \{\Delta\lambda_k,\ \Delta\Psi_k\}$:

$$\begin{array}{l} (H - \lambda_k I)\Delta\Psi_k = -(H - \lambda_k I)\Psi_k + \Delta\lambda_k\Psi_k, \\ F'_\lambda(\lambda_k, \Psi_k)\Delta\lambda_k + F'_\Psi(\lambda_k, \Psi_k)\Delta\Psi_k = -F(\lambda_k, \Psi_k). \end{array} \tag{10}$$

Depending on the method of solving this system and the choice of the form of functional F, it is possible to receive various known iteration schemes for solving the spectral problems. Representing $\Delta\Psi_k$ in the form

$$\Delta\Psi_k = -\Psi_k + \Delta\lambda_k U_k, \tag{11}$$

where U_k is a solution of the problem

$$(H - \lambda_k I)U_k = \Psi_k,$$

we receive the following expression for $\Delta\lambda_k$:

$$\Delta\lambda_k = \frac{1 + (\Psi_k,\ \Psi_k)}{2(\Psi_k,\ U_k)}.$$

At $\tau_k = 1$ we receive the following expression for new approximations

$$\begin{array}{l} \Psi_{k+1} = \Delta\lambda_k (H - \lambda_k I)^{-1}\Psi_k, \\ \lambda_{k+1} = \lambda_k + \frac{1+(\Psi_k,\ \Psi_k)}{2(\Psi_k,\ (H-\lambda_k I)^{-1}\Psi_k)}. \end{array} \tag{12}$$

One can see that we have received a known scheme of inverse iterations.

When using functional F in the form Eq (9 b), we receive the following system with respect to the iterative corrections

$$(H - \lambda_k I)\Delta\Psi_k - \Delta\lambda_k\Psi_k = -(H - \lambda_k I)\Psi_k,$$

$$(\Delta\Psi_k(, H - \lambda_k I)\Psi_k) + (\Psi_k, (H - \lambda_k I)\Delta\Psi_k) - (\Psi_k, \Delta\lambda_k\Psi_k) = -(\Psi_k, (H - \lambda_k I)\Psi_k).$$

Using the first equation of this system, we receive from the second equation

$$(\Delta\Psi_k, (H - \lambda_k I)\Psi_k) = 0.$$

If the operator H is self-conjugate, then

$$(\Psi_k, (H - \lambda_k I)\Delta\Psi_k) = 0. \tag{13}$$

Substitution of the expression for $\Delta\Psi_k$

$$\Delta\Psi_k = -\Psi_k + \Delta\lambda_k (H - \lambda_k I)^{-1}\Psi_k \tag{14}$$

in relation Eq (13) gives

$$-(\Psi_k, (H - \lambda_k I)\Psi_k) + \Delta\lambda_k (\Psi_k, \Psi_k) = 0.$$

Thus, we have for $\tau_k = 1$

$$\Delta\lambda_k (\Psi_k, \Psi_k) = (\Psi_k, H\Psi_k) - \lambda_k (\Psi_k, \Psi_k),$$

or

$$\begin{array}{l} \Psi_{k+1} = \Delta\lambda_k (H - \lambda_k I)^{-1}\Psi_k, \\ \lambda_{k+1} = \frac{(\Psi_k, H\Psi_k)}{(\Psi_k, \Psi_k)}. \end{array} \tag{15}$$

This formula together with expression Eq (12) for approximation λ_{k+1} leads to a known scheme of the inverse iterations with Rayleigh's shift.

In addition to the continuous analogue of the Newton's method, it is possible to consider a continuous analogue of the modified Newton's method. It is represented by an evolution process

$$\varphi'(a, \tilde{z}(t))\frac{dz(t)}{dt} = -\varphi(a, z(t)), \tag{16}$$

$$z(0) = z_0, \tag{17}$$

where $\tilde{z}$ is a fixed element from the neighborhood of the required solution z^*. This approach gives the iteration schemes Eq (7), in which the operator $\varphi'(a, \tilde{z}(t))$ is required to be converted only once. In the spectral problems, when the unknown z consists of two-components λ and Ψ, and both or one of these components, can be fixed depending on how well we know a corresponding approximation to the required solution. For example, at the fixed value $\lambda_k = \tilde{\lambda}$ from the system Eq (10) with functional F in the form Eq (9 a) we receive

$$(H - \tilde{\lambda} I)\Delta\Psi_k = -(H - \lambda_k I)\Psi_k + \Delta\lambda_k \Psi_k, \tag{18}$$

$$2(\Psi_k, \Delta\Psi_k) = 1 - (\Psi_k, \Psi_k). \tag{19}$$

Solution to equation Eq (18) can be given in the form

$$\Delta\Psi_k = v_k + \Delta\lambda_k w_k. \tag{20}$$

Thus v_k is equal to

$$v_k = -\Psi_k - (H - \tilde{\lambda} I)^{-1}(\tilde{\lambda} - \lambda_k)\Psi_k, \tag{21}$$

and w_k is equal to

$$w_k = (H - \tilde{\lambda} I)^{-1}\Psi_k. \tag{22}$$

Substituting expressions Eq (21) and Eq (22) in Eq (20) we receive

$$\Delta\Psi_k = -\Psi_k + (\lambda_{k+1} - \tilde{\lambda})(H - \tilde{\lambda} I)^{-1}\Psi_k.$$

For $\tau_k = 1$ we have

$$\begin{array}{l} \Psi_{k+1} = (\lambda_{k+1} - \tilde{\lambda})(H - \lambda_k I)^{-1}\Psi_k, \\ \lambda_{k+1} = \tilde{\lambda} + \frac{1 + (\Psi_k,\ \Psi_k)}{2(\Psi_k,\ (H - \tilde{\lambda} I)^{-1}\Psi_k)}. \end{array} \tag{23}$$

This is a scheme of inverse iterations with a fixed shift. This scheme can be used in combination with orthogonalization of the found approximation Ψ_{k+1} to all already found eigenelements $\{\Psi_m^*\}$, where m is the number of the eigenelement, provided this set is an orthogonal system with some weight.

3 Formulation of the scattering problem as an eigenvalue problem and a stable iteration scheme

1. One can see that the scattering problem for the radial Schrödinger equation on the semiaxis $0 < r < \infty$ with short-range potential $V(r)$ for a given impulse k has the form

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2\right)\Psi(r) = 2V(r)\Psi(r), \tag{24}$$

which consists in finding regular solutions $\Psi(r)$ with asymptotic conditions

$$\Psi(r) \approx r^l, \ r \to 0, \tag{25}$$

$$\Psi(r) \approx A\frac{\sin(kr - \pi l/2 + \delta_l)}{r}, \ r \to \infty, \tag{26}$$

and calculating phase δ_l. Here l is the orbital moment. If $A = (k\cos\delta_l)^{-1}$ and the regular solutions $\Psi(r)$ with asymptotics is written as

$$\Psi(r) \approx \frac{\sin(kr - \pi l/2) + \cos(kr - \pi l/2)tg\delta_l}{kr}, \ r \to \infty, \tag{27}$$

the regular solutions are represented by the form [1, 2]

$$\Psi(r) = j_l(kr) - 2k\int_0^\infty j_l(kr_<)h_l^+(kr_>)V(r')\Psi(r')r'^2dr', \tag{28}$$

where

$$h_l^+(r) = -y_l(r) + ij_l(r), \ r_< = \min\{r, r'\}, \ r_> = \max\{r, r'\}, \tag{29}$$

$j_l(r)$ is a Bessel spherical function, $y_l(r)$ is a Neumann function.

The asymptotics of solution $\Psi(r)$ at $r \to \infty$ has the form

$$\Psi(r) \longrightarrow j_l(kr) - 2k\int_0^\infty j_l(kr')V(r')\Psi(r')r'^2dr'h_l^+(kr). \tag{30}$$

We denote

$$\nu_l^{-1}(\delta_l) = 2\int_0^\infty j_l(kr')V(r')\Psi(r')r'^2dr'. \tag{31}$$

By means of this expression we can write the following identity

$$\begin{array}{l}\Psi(r) + 2k\int_0^\infty j_l(kr_<)h_l^+(kr_>)V(r')\Psi(r')r'^2dr' = \\ \quad = j_l(kr)\nu_l(\delta_l)2\int_0^\infty j_l(kr')V(r')\Psi(r')r'^2dr',\end{array} \tag{32}$$

or

$$\begin{array}{l}\Psi(r) - 2k\int_0^\infty j_l(kr_<)y_l(kr_>)V(r')\Psi(r')r'^2dr' = \\ \quad = \lambda(\delta_l)2j_l(kr)\int_0^\infty j_l(kr')V(r')\Psi(r')r'^2dr'.\end{array} \tag{33}$$

Here

$$\lambda(\delta_l) \equiv -kctg\delta_l = \nu_l(\delta_l) - ik \tag{34}$$

is the value of the required phase shift $\delta_l = \delta_l(k)$ is defined at a fixed value of momentum k.

Let us introduce integral operators

$$\begin{array}{l}A(r, r')\Psi(r) = \Psi(r) - 2k\int_0^\infty j_l(kr_<)y_l(kr_>)V(r')\Psi(r')r'^2dr', \\ B(r, r')\Psi(r) = 2j_l(kr)\int_0^\infty j_l(kr')V(r')\Psi(r')r'^2dr'.\end{array} \tag{35}$$

Then Eq (33) takes the form

$$(A(r,r') - \lambda B(r,r'))\Psi(r') = 0, \tag{36}$$

where $\lambda = -kctg\delta_l$ is a spectral parameter. Let us add the condition of orthogonality to Eq (36):

$$F(\lambda,\Psi) = (\Psi(r)V(r)r^2, (A(r,r') - \lambda B(r,r'))\Psi(r')) = 0. \tag{37}$$

From this condition of orthogonality it follows that

$$\lambda = \frac{(\Psi(r)V(r)r^2, A(r,r')\Psi(r'))}{(\Psi(r)V(r)r^2, B(r,r')\Psi(r'))}. \tag{38}$$

This formula is analogous to the Rayleigh relation in the discrete spectrum problem of the energy operator. However, it only has a property of stationary state, not extreme state. As opposed to the standard formulations of the scattering problem, Eqs (36), (37) allow one to formulate the spectral problem with respect to the pair $z = \{\lambda, \Psi\}$, the eigenelement Ψ being accurate within the constant:

$$\varphi(z) = \left\{ \begin{array}{l} (A - \lambda B)\Psi \\ (\Psi V r^2, (A - \lambda B)\Psi) \end{array} \right\} = 0. \tag{39}$$

The evolution equation Eq (4) for this problem takes the form

$$(A - \lambda B)\frac{d\Psi}{dt} - B\Psi\frac{d\lambda}{dt} = -(A - \lambda B)\Psi. \tag{40}$$

If the operator $V(A - \lambda B)\Psi$ is a self-conjugate one and the condition,

$$(\Psi r^2, V(A - \lambda B)\Psi) = (\Psi V r^2, (A - \lambda B)\Psi),$$

is fulfilled, then the following relation takes place:

$$\begin{array}{c} \left(\Psi r^2, V(A - \lambda B)\frac{d\Psi}{dt}\right) + \left(\Psi r^2, V\left((A - \lambda B)\frac{d\Psi}{dt} - B\Psi\frac{d\lambda}{dt}\right)\right) = \\ = -(\Psi r^2, V(A - \lambda B)\Psi). \end{array} \tag{41}$$

Using equation Eq (40) in Eq (41), we have

$$\left(\Psi r^2, V(A - \lambda B)\frac{d\Psi}{dt}\right) = 0. \tag{42}$$

Then, using the standard representation of the derivative

$$\frac{d\Psi}{dt} = \frac{\partial\Psi}{\partial t} + \frac{\partial\Psi}{\partial\lambda}\frac{d\lambda}{dt}, \tag{43}$$

we have from Eq (40)the following equations for corrections

$$\left\{ \begin{array}{l} \frac{\partial\Psi}{\partial t} = -\Psi \\ (A - \lambda B)\frac{\partial\Psi}{\partial\lambda} = B\Psi. \end{array} \right. \tag{44}$$

Substituting Eq (43) and Eq (44) in the ratio Eq (42), we get

$$\frac{d\lambda}{dt} = \frac{(\Psi V r^2, (A - \lambda B)\Psi)}{(\Psi V r^2, B\Psi)}, \tag{45}$$

or in an integral form

$$\frac{d\lambda}{dt} = -\frac{2k\int_0^\infty\int_0^\infty \Psi(r)V(r)j_l(kr_<)y_l(kr_>)V(r')\Psi(r')r'^2r^2dr'dr}{2\left(\int_0^\infty j_l(kr')V(r')\Psi(r')r'^2dr'\right)^2} + \\ + \frac{\int_0^\infty \Psi_l^2(r)V(r)r^2dr}{2\left(\int_0^\infty j_l(kr')V(r')\Psi(r')r'^2dr'\right)^2} - \lambda. \tag{46}$$

The functional of the right-hand side of Eq (46) corresponds to Schwinger variational functional Eq (1).

At discrete representation, expression Eq (33) takes the form

$$\tilde{\Psi}(r_i) - 2k\sum_{j=1}^N G_{ij}V(r_j)r_j^2\xi_j\tilde{\Psi}(r_j) = \\ = \overline{\lambda}(\delta_l)2j_l(kr_i)\sum_{j=1}^N j_l(kr_j)V(r_j)r_j^2\xi_j\tilde{\Psi}(r_j),\ i=\overline{1,n}, \tag{47}$$

where ξ_j are coefficients of the quadrature formula and r_j are nodes,

$$G_{ij} = j_l(k\min\{r_i,r_j\})y_l(k\max\{r_i,r_j\}).$$

Then we can write

$$(\overline{A} - \overline{\lambda}\ \overline{B})\tilde{\Psi}(r) = 0, \tag{48}$$

where

$$\{\overline{A}\}_{ij} = \delta_{ij} - 2kG_{ij}V(r_j)r_j^2\xi_j \tag{49}$$

$$\{\overline{B}\}_{ij} = 2j_l(kr_i)j_l(kr_j)V(r_j)r_j^2\xi_j. \tag{50}$$

In this case, we obtain the following iteration scheme:

$$\begin{cases} v_n = -\Psi_n, \\ (\overline{A} - \overline{\lambda}_n\overline{B})u_n = \overline{B}\Psi_n, \\ \mu_n = \frac{(\Psi_n Vr^2,\ \overline{A}\Psi_n)}{(\Psi_n Vr^2,\ \overline{B}\Psi_n)} - \lambda_n, \\ \Psi_{n+1} = \Psi_n + \tau_n(v_n + u_n\mu_n), \\ \overline{\lambda}_{n+1} = \overline{\lambda}_n + \tau_n\mu_n, \end{cases} \tag{51}$$

where $n = 0,1,2,\ldots$; $\{\lambda_0,\ \Psi_0\}$ are predetermined. In order to choose an iterative step τ_n, we use a method based on minimization of the residual [8]. A new program package JINRLINPACK [11] was used for numerical solving the actually ill-conditioned ($0.41\cdot 10^7 \le cond \le 0.30\cdot 10^{10}$) system Eq (51).

2. Let us consider separately the elastic scattering problem for a one-dimensional Schrödinger equation along the whole axis $(-\infty,\infty)$ with short-range potential $V(x)$ for a given impulse k

$$\left(\frac{d^2}{dx^2} + k^2\right)\Psi(x) = 2V(x)\Psi(x), \tag{52}$$

which consists of determination of regular solutions $\Psi(x)$ with asymptotic conditions

$$\Psi(x) \approx 0,\ x\to -\infty, \tag{53}$$

$$\Psi(x) \approx A\sin(kx+\delta),\ x\to\infty, \tag{54}$$

and calculation of phase shifts δ. In this case, it is difficult to write down the solution in an integrated form by means of the first boundary conditions Eq (53). We consider the following boundary condition in the place of Eq (53)

$$\Psi(x) \to 0,\ x\to a,\ a<0. \tag{55}$$

Then the regular solutions are represented in the form

$$\Psi(x) = \sin(k(x-a)) - \frac{2}{k\cos(ka)} \int_a^\infty \sin(k(x_< - a)) \times \\ \times \cos(kx_>) V(x') \Psi(x') dx'. \tag{56}$$

Here $x_< = \min\{x, x'\},\ x_> = \max\{x, x'\}$. The asymptotics of solution $\Psi(x)$ have the form:

$$\Psi(x) \longrightarrow 0,\ x \to a; \tag{57}$$

$$\Psi(x) \longrightarrow \sin(k(x-a)) - \frac{2}{k\cos(ka)} \cos(kx) \int_a^\infty \sin(k(x'-a)) \times \\ \times V(x') \Psi(x') dx',\ x \to \infty. \tag{58}$$

Let us denote

$$\nu(\delta) = -\frac{2}{k\cos(ka)} \int_a^\infty \sin(k(x'-a)) V(x') \Psi(x') dx'. \tag{59}$$

We can write the following identity by means of this expression:

$$\Psi(x) + \frac{2}{k\cos(ka)} \int_a^\infty \sin(k(x_< - a)) \cos(kx_>) V(x') \Psi(x') dx' = \\ = \lambda(\delta) \frac{2}{k\cos(ka)} \sin(k(x-a)) \int_a^\infty \sin(k(x'-a)) V(x') \Psi(x') dx'. \tag{60}$$

Here

$$\lambda(\delta) = -1/\nu(\delta) = \frac{-1}{\cos(ka) tg(\delta) + \sin(ka)} \tag{61}$$

defines the value of the required phase shift $\delta = \delta(k)$. Thus $A = \frac{\cos(ka)}{\cos(\delta)}$. We can use the proposed method in that follows.

4 Numerical examples and discussions

To analyze the accuracy of the calculation procedure, it is convenient to consider examples with known analytical solutions.

4.1 The Morse potential

Let us consider Eq (52) with the Morse potential [9]

$$V(x) = MD \left(e^{-2\alpha(x-x_\alpha)} - 2e^{-\alpha(x-x_\alpha)} \right). \tag{62}$$

Analytical solution $\Psi(x)$, corresponding to the continuous spectrum $k > 0$, has the form [10]

$$\Psi(x) = e^{-0.5\xi} Im \left(e^{i\omega} \xi^{-is} F(-d + 0.5 - is, 1 - 2is, \xi) \right), \tag{63}$$

where F is a confluence-hypergeometric function,

$$\xi = 2de^{-\alpha(x-x_\alpha)},\ d = \frac{\sqrt{2MD}}{\alpha},\ s = \frac{k}{\alpha}, \\ \omega = arg\Gamma(1+2is) + arg\Gamma(-d+0.5-is), \tag{64}$$

and Γ is a gamma-function.

One of the peculiarities of the considered problem is that the independent variable x changes along the entire axes $-\infty < x < \infty$, and

$$V(x) \longrightarrow +\infty,\ x \to -\infty,\quad V(x) \longrightarrow 0,\ x \to \infty \tag{65}$$

and function $\Psi(x)$ has asymptotics of the form

$$\Psi(x) \longrightarrow 0, x \to -\infty,\quad \Psi(x) \longrightarrow \sin(kx + \delta),\ x \to \infty. \tag{66}$$

Here the required phase shift δ takes the form

$$\delta = -kx_\alpha - s\ln(2d) + \omega. \tag{67}$$

The results of two calculations with boundary conditions Eq (25) and Eq (53) permitting to evaluate the contribution of potential $V(x)$ on the segment $x \in [-a, 0]$ to the solution are given below.

k	$h = 0.1$	$h/2$	$h/4$	$h \to 0$	$-\delta$[5]
0.20	1.2599077	1.2618001	1.2622719	1.2624285	1.262287
0.14	0.9000893	0.9015871	0.9019605	0.9020844	0.9019789
0.10	0.6495453	0.6506877	0.6509724	0.6510669	0.6509868
0.08	0.5217001	0.5226381	0.5228720	0.5229496	0.5228852
$1.0A$	$6.568483A$	$6.580794A$	$6.583863A$	$6.584882A$	$6.58407A$

Table 1. Phases of scattering $-\delta$; $x \in (0, 35)$, $A = 10^{-4}$

k	$h = 0.1$	$h/2$	$h/4$	$h \to 0$	$-\delta_{AH}$
0.20	1.2557224	1.2576763	1.2581631	1.2583246	1.2583252
0.14	0.8968501	0.8983957	0.8987808	0.8989086	0.8989090
0.10	0.6471009	0.6482795	0.6485731	0.6486705	0.6486709
0.08	0.5197008	0.5206686	0.5209097	0.5209897	0.5209899
$1.0A$	$6.542430A$	$6.555129A$	$6.558293A$	$6.559343A$	$6.559345A$

Table 2. Phases of scattering $-\delta$; $x \in (-5, 35)$, $A = 10^{-4}$

In a numerical example, the values of parameters

$$M = 8.876,\ D = 0.104,\ \alpha = 0.67,\ x_\alpha = 2.09 \tag{68}$$

correspond to the values of parameters in [5]. This potential is given in Figure 1. The accuracy of the numerical results depends on the parameters of difference grid $\Omega_h = \{x_{\min} = x_0;\ x_j = x_0 + jh;\ j = \overline{1, N};\ x_n = x_{\max}\}$. Table 1 and Table 2 give the numerical results of the quantity $-\delta$, for calculation of which the formulas Eq (28) and Eq (56), respectively, were used. The contribution of the interval $x \in [-5, 0]$ to δ is a value of the order 10^{-2}. Convergence of difference solutions δ_h corresponds to theoretical one $O(h^2)$, as the quantity

$$\sigma = (\delta_h - \delta_{h/2})/(\delta_{h/2} - \delta_{h/4}) \approx 4. \tag{69}$$

In Table 2, the extrapolated values of quantity $-\delta$ are compared to the analytical values $-\delta_{AH}$ computed by formula Eq (67). The analysis of the results show that for $h \to 0$ the extrapolation ensures the accuracy of calculating the phase shift $\approx 10^{-5} \div 10^{-6}$. Figure 2 shows the precise solution and the numerical solutions $\Psi(x)$ for $k = 0.2$. They are in a good agreement.

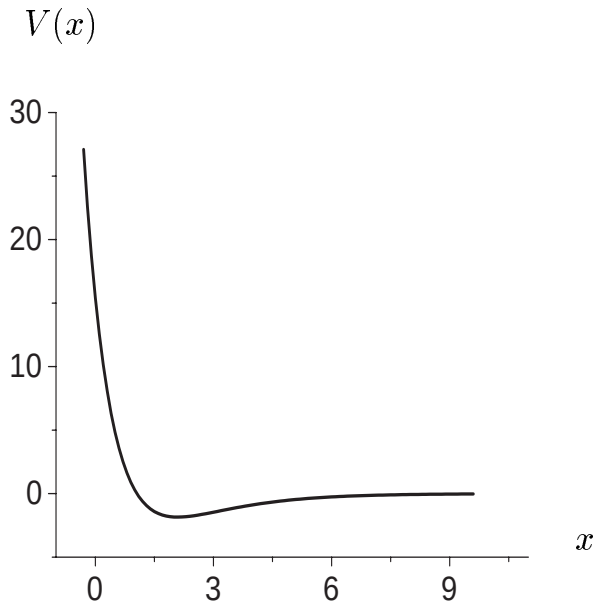

Figure 1: An aspect of a potential the Morse $V(x)$ with parameters M=8.876, D=0.104, α=0.67, x_α=2.09.

4.2 The potential of the spherical well

Let us consider Eq (24) for $l = 0$ with a potential spherical well

$$V(r) = \begin{cases} -V_0 < 0, & r < r_0 \\ 0, & r > r_0 \end{cases} . \tag{70}$$

Analytical solution $\Psi(r)$ for $k \to 0$ on the interval $r \in (0, r_0)$ takes the form:

$$\Psi_0(r) \longrightarrow \frac{1}{\cos(\sqrt{2V_0}r_0)} \frac{\sin(\sqrt{2V_0}r)}{\sqrt{2V_0}r}. \tag{71}$$

The value of the scattering length a_0 is defined δ_0 by formula

$$a_0 = -\lim_{k\to 0}(kctg(\delta_0)) = -\left(\left(\frac{tg(\sqrt{2V_0}r_0)}{\sqrt{2V_0}r_0)} - 1\right) r_0\right)^{-1}. \tag{72}$$

b_0	$h = 0.02$	$h/2$	$h/4$	$h \to 0$	a_0^{AH}
0.2π	−6.3966702	−6.3967619	−6.3967848	−6.3967924	−6.3967925
0.4π	−0.6899402	−0.6900324	−0.6900554	−0.6900630	−0.6900631
0.6π	0.3799557	0.3798608	0.3798371	0.3798292	0.3798292
0.8π	0.7758865	0.7757809	0.7757545	0.7757457	0.7757457
1.0π	1.0002012	1.0000502	1.0000125	1.0000000	1.0000000

Table 3. Numerical results for a_0, $r \in (0, 1)$; k=1. E-5

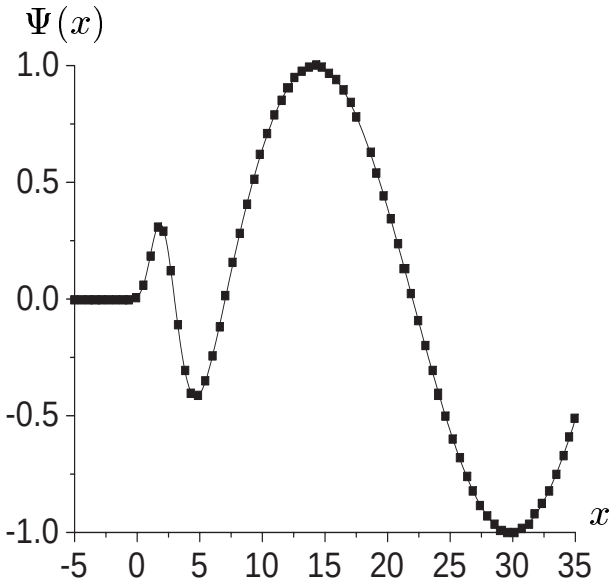

Figure 2: An aspect function $\Psi(x)$ at k=0.20. The full-line by the formula Eq (63), the dashed-line numerical result.

b_0	$h = 0.02$	$h/2$	$h/4$	$h \to 0$	a_0^{AH}
0.2π	-6.3968484	-6.3969401	-6.3969630	-6.3969706	-6.3967925
0.4π	-0.6900041	-0.6900963	-0.6901193	-0.6901269	-0.6900631
0.6π	0.3799134	0.3798186	0.3797949	0.3797870	0.3798292
0.8π	0.7758527	0.7757471	0.7757207	0.7757119	0.7757457
1.0π	1.0001730	1.0000220	0.9999843	0.9999717	1.0000000

Table 4. Numerical results for a_0, $r \in (0, 1)$; k=1. E-2

In this example it is enough to compute a_0 on the interval $(0 \leq r \leq r_0)$. Let us denote $b_0 = \sqrt{2V_0}r_0$ and in calculation use $r_0 = 1$. Table 3 and Table 4 show the numerical results of the value a_0 obtained when using the formula Eq (28). The convergence of difference solutions δ_h corresponds to the theoretical value $O(h^2)$

$$\sigma = (\delta_h - \delta_{h/2})/(\delta_{h/2} - \delta_{h/4}) \approx 4. \tag{73}$$

In Table 3 and Table 4 the extrapolated values of a_0 are compared with the analytical values of a_0^{AH}, computed by formula Eq (72). The analysis of the results shows that extrapolation for $h \to 0$ ensures the accuracy of calculating $a_0 \approx 10^{-6} \div 10^{-7}$ for $k = 1.E-5$ and $\approx 10^{-3}$ for $k = 1.E-2$. Figure 3 gives the matching of the precise solution and the numerical solution $\Psi(x)$ for $b_0 = \pi$. They are in a good agreement.

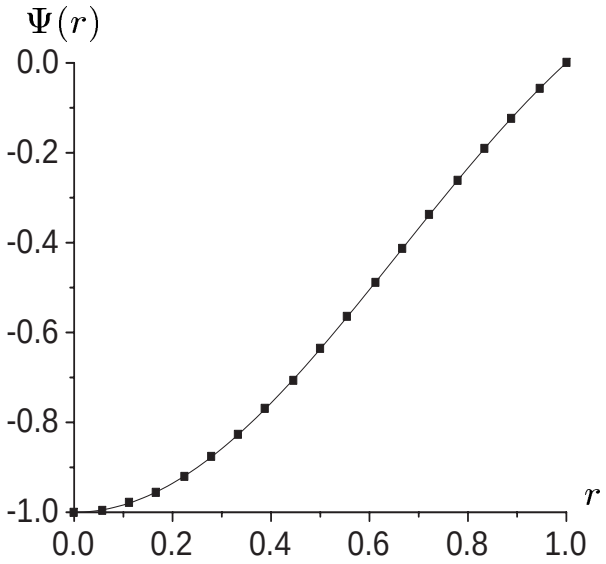

Figure 3: An aspect a function $\Psi(r)$, at $b_0 = \pi$ and k=1. E-5. A full-line by the formula Eq (71), dashed-line numerical result.

5 Conclusion

To solve the scattering problem with a predetermined accuracy, a stable iteration scheme is constructed on the basis of CANM. The scattering problem is formulated as an eigenvalue problem with respect to a pair of unknowns: a phase shift and a wavefunction using the Schwinger variational functional. The efficiency of the proposed iteration scheme is demonstrated on precisely solved examples of elastic scattering with Morse and spherical well potentials. The proposed approach allows a direct generalization of many-dimensional and multi-channel scattering problems at an eligible choice of approximation of solutions, for example, by means of separable potentials, Bateman approximations, as well as by the way of trial functions with given variational parameters in the scope of the potential. Outside this field, asymptotic states with an unknown scattering amplitude are given, the parameters of which are found by means of the proposed iteration scheme.[1]

Acknowledgment

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