Newtonian iteration schemes for solving the three-boson scattering problem on a line

O. Chuluunbaatar[a], I.V. Puzynin[a], D.V. Pavlov[a], A.A. Gusev[a], S.Y. Larsen[b] and S.I. Vinitsky[c]

[a] Laboratory of Information Technologies, Joint Institute for Nuclear Research, Dubna, Moscow Region 141980, Russia
[b] Temple University, Philadelphia, PA 19122, USA
[c] Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, Moscow Region 141980, Russia

ABSTRACT

A three-body scattering problem is formulated in an adiabatic representation as a multichannel spectral problem for a system of one-dimensional integral equations using the Schwinger variational functional. The stable Newtonian iteration schemes for calculating the eigenfunctions and eigenvalues which are phase shift and energy for continuous and discrete spectrum, correspondingly, are elaborated. Convergence and efficiency of the proposed schemes are demonstrated using the exact solvable model of three identical particles (bosons) on a line with pair attractive δ-potentials.

Keywords: newtonian iteration schemes, Schwinger variational functional, three-boson scattering problem

1. INTRODUCTION

In nuclear and atomic physics the scattering problems are connected with the calculations of a scattering amplitude, phase shifts and mixing parameters, comprising the definition of the asymptotic wave functions obeying to the Schrödinger equation with the pair short-range potentials $\mathbf{V}$[1] and with an effective long-range potentials.[2] To solve the scattering problem different methods are used. One of the common approaches is the Schwinger variational method based on the following expression for the variational functional[3]:

$$f(\mathbf{k},\mathbf{k}') = -\frac{1}{2\pi}\frac{(\mathbf{k}'|\mathbf{V}|\eta_{\mathbf{k}}^{(+)})(\eta_{\mathbf{k}'}^{(-)}|\mathbf{V}|\mathbf{k})}{(\eta_{\mathbf{k}'}^{(-)}|\mathbf{V}-\mathbf{V}\mathbf{G}_0\mathbf{V}|\eta_{\mathbf{k}}^{(+)})}. \qquad (1)$$

Here $|\eta)$ are the basis functions, G_0 is the Green function. It allows to calculate amplitudes and scattering phases more accurately than in Born approximation.[4] It was shown,[5,6] that it is possible to find effectively the solutions of a scattering problem using different iteration schemes constructed on the basis of Schwinger variational functional Eq. (1), utilizing the separable approximation for the short-range potential

$$\begin{cases} V^{(N)} = \sum_{i,j=1}^{N} V|\eta_i)d_{ij}^{(N)}(\eta_j|V; \\ d_{ij}^{-1} = (\eta_i|V|\eta_j). \end{cases} \qquad (2)$$

Nevertheless, the problems of construction the stable iteration schemes permitting calculations of the solutions with predetermined accuracy, are still actual.

In the paper,[7] the stable iteration scheme has been constructed for the solution of the scattering problem for Schrödinger equation based on the Continuous Analogue of Newton's Method (CANM), using the additional Hulthen variational functional. In present paper, the CAMN is applied to solve a multichannel scattering problem with a predetermined accuracy in the framework of the system of integral equations and using the additional Schwinger variational functional Eq. (1). Convergence and efficiency of the proposed schemes are demonstrated for the exact solvable model of three identical particles on a line with pair attractive δ-potentials.[8]

Further author information:
S.I.V.: E-mail: vinitsky@thsun1.jinr.ru

2. THE THREE-BOSON PROBLEM IN ADIABATIC REPRESENTATION

We consider three identical particles in the local Jacobi coordinates $\{\xi, \eta\} \in R^2$ in the center-of-mass reference-frame-system:

$$\begin{aligned} \eta &= \left(\tfrac{1}{2}\right)^{1/2}(x_1 - x_2), \\ \xi &= \left(\tfrac{2}{3}\right)^{1/2}\left[\left(\tfrac{x_1+x_2}{2}\right) - x_3\right], \end{aligned} \tag{3}$$

where $\{x_1, x_2, x_3\} \in R^1$ are the Cartesian coordinates of the particles on a line. In polar coordinates ρ and θ

$$\eta = \rho\cos\theta, \;\; \xi = \rho\sin\theta, \;\; -\pi \le \theta \le \pi, \tag{4}$$

the Schrödinger equation for a partial wave function $\Psi(\rho, \theta)$ has the form:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}\right]\Psi(\rho,\theta) + V(\rho,\theta)\Psi(\rho,\theta) = E\Psi(\rho,\theta). \tag{5}$$

Here E is the relative energy in the center-of-mass coordinate system, $m = (m_1m_2 + m_1m_3 + m_2m_3)/(m_1 + m_2 + m_3)$ is the effective mass, the potential function $V(\rho, \theta)$ is defined as the sum of the pair potentials

$$V(\rho,\theta) = V(\sqrt{2}\rho|cos\theta|) + V(\sqrt{2}\rho|\cos(\theta - 2\pi/3)|) + V(\sqrt{2}\rho|\cos(\theta + 2\pi/3)|). \tag{6}$$

We choose these pair potentials $V(\sqrt{2}\eta) = g\delta(|\eta|)/\sqrt{2}$ as delta-functions of a finite strength $g = c\bar{k}\sqrt{2}(\hbar^2/m)$, and consider an attractive case $c = -1$ and $\bar{k} = \pi/6$.

Let us select h_ρ- the parametric Hamiltonian at each fixed value $\rho \in R^1_+$ (in a.e. $\hbar = m = 1$):

$$h_\rho = -\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2} + \frac{2c\bar{k}}{\rho}\sum_n \delta(\theta - \theta_n), \quad \theta_n = n\pi/3 + \pi/6, \; n = 0, 1, ...5. \tag{7}$$

The complete set of the orthogonal adiabatic functions $B_j(\rho, \theta) \in L_2(C)$ includes the solutions of the eigenvalue problem on circle $C(-\pi \le \theta \le \pi)$

$$\begin{aligned} h_\rho B_j(\rho,\theta) &= \epsilon_j(\rho)B_j(\rho,\theta) \\ < B_i(\rho,\theta)|B_j(\rho,\theta) > &= \int_{-\pi}^{\pi} B_i^*(\rho,\theta)B_j(\rho,\theta)d\theta = \delta_{ij}. \end{aligned} \tag{8}$$

The corresponded boundary problems for calculation $\epsilon_j(\rho), B_j(\rho, \theta)$ may be written as follows:

$$\left\{ \begin{array}{rcl} \dfrac{\partial^2 B_0(\rho,\theta)}{\partial\theta^2} &=& \Big(6y_0(\rho)\Big)^2 B_0(\rho,\theta), \\ \dfrac{1}{\rho}\dfrac{\partial B_0(\rho,\theta)}{\partial\theta}\Bigg|_{\theta=-\frac{\pi}{6}+\frac{\pi n}{3}} &=& \dfrac{c\pi}{6}B_0(\rho,\theta)\Bigg|_{\theta=-\frac{\pi}{6}+\frac{\pi n}{3}}, \\ \dfrac{1}{\rho}\dfrac{\partial B_0(\rho,\theta)}{\partial\theta}\Bigg|_{\theta=\frac{\pi}{6}+\frac{\pi n}{3}} &=& -\dfrac{c\pi}{6}B_0(\rho,\theta)\Bigg|_{\theta=\frac{\pi}{6}+\frac{\pi n}{3}}, \end{array} \right. \tag{9}$$

$$\left\{ \begin{array}{rcl} -\dfrac{\partial^2 B_j(\rho,\theta)}{\partial\theta^2} &=& \Big(6y_j(\rho)\Big)^2 B_j(\rho,\theta), \\ \dfrac{1}{\rho}\dfrac{\partial B_j(\rho,\theta)}{\partial\theta}\Bigg|_{\theta=-\frac{\pi}{6}+\frac{\pi n}{3}} &=& \dfrac{c\pi}{6}B_j(\rho,\theta)\Bigg|_{\theta=-\frac{\pi}{6}+\frac{\pi n}{3}}, \\ \dfrac{1}{\rho}\dfrac{\partial B_j(\rho,\theta)}{\partial\theta}\Bigg|_{\theta=\frac{\pi}{6}+\frac{\pi n}{3}} &=& -\dfrac{c\pi}{6}B_j(\rho,\theta)\Bigg|_{\theta=\frac{\pi}{6}+\frac{\pi n}{3}}. \end{array} \right. \tag{10}$$

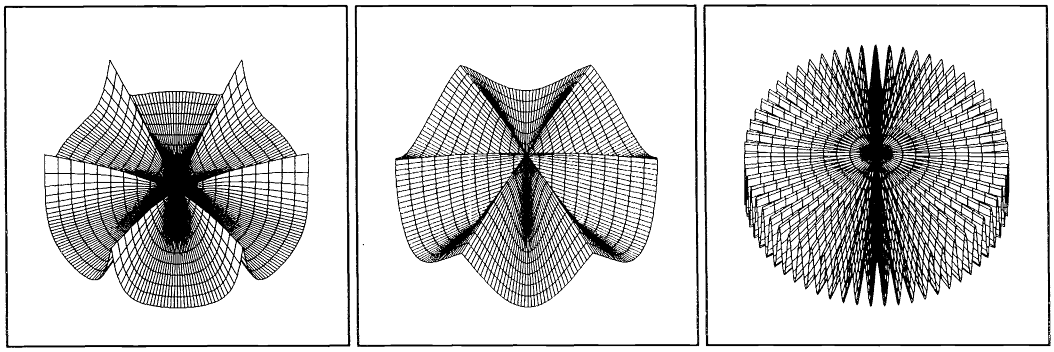

Figure 1: The orthogonal adiabatic functions $B_j(\rho,\theta)$.

The set of eigenfunctions symmetrical against interchanging of the particles including the basis states for six sectors of circle (see Fig. 1)

$$\begin{aligned} B_0(\rho,\theta) &= \sqrt{\frac{y_0^2-x^2}{\pi(y_0^2-x^2)+|x|}}\cosh\left[6y_0(\theta-n\pi/3)\right], \\ B_j(\rho,\theta) &= \sqrt{\frac{y_j^2+x^2}{\pi(y_j^2+x^2)-|x|}}\cos\left[6y_j(\theta-n\pi/3)\right], \end{aligned} \tag{11}$$

has been proposed[8] for

$$n\pi/3-\pi/6 \le \theta \le n\pi/3+\pi/6,\ n=0,1,...5. \tag{12}$$

The eigenvalues $\epsilon_0(\rho)$ and $\epsilon_j(\rho), j=1,2,3,...$ are determined via the reduced eigenvalues $y_0(\rho)$ and $y_j(\rho), j=1,2,3,...$,

$$\epsilon_0(\rho) = -\left(\frac{6y_0(\rho)}{\rho}\right)^2,\ \epsilon_j(\rho) = \left(\frac{6y_j(\rho)}{\rho}\right)^2. \tag{13}$$

The roots $y_0(\rho)$ and $y_j(\rho), j=1,2,3,...$, are the solutions of transcendental equations, which follow from the boundary problems (9, 10):

$$\begin{aligned} y_0(\rho)\tanh(\pi y_0(\rho)) = -x,\ 0\le y_0(\rho)<\infty,\quad x=c\tfrac{\pi}{36}\rho,\ c=-1, \\ y_j(\rho)\tan(\pi y_j(\rho)) = x,\ j-\tfrac{1}{2}<y_j(\rho)<j,\ j=1,2,3,.... \end{aligned} \tag{14}$$

The eigenvalue $\epsilon_j(\rho)$ has following asymptotic behaviour for large ρ:

$$\epsilon_0^{(0)} = \lim_{\rho\to\infty}\epsilon_0(\rho) = -\frac{\pi^2}{36},\ \epsilon_j(\rho)|_{\rho\to\infty} \to \left(\frac{6(j-1/2)}{\rho}\right)^2 \tag{15}$$

and for small ρ

$$\epsilon_0(\rho)|_{\rho\to0} \to -\frac{1}{\rho}\left(1+\frac{\pi^2}{108}\rho+\frac{\pi^4}{14580}\rho^2\right),\ \epsilon_j(\rho)|_{\rho\to0} \to \left(\frac{6j}{\rho}\right)^2. \tag{16}$$

Let us express the wave function $\Psi(\rho,\theta)$ in terms of complete orthogonal set of adiabatic functions $B_j(\rho,\theta)$

$$\Psi(\rho,\theta) = \sum_{j=0}^{\infty}\chi_j(\rho)B_j(\rho,\theta). \tag{17}$$

As the result of projection of Eq. (5) onto $B_j(\rho,\theta)$, we obtain the system of coupled adiabatic equations

$$\left(\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho}+2E-\epsilon_i(\rho)\right)\chi_i(\rho) = \sum_{j=0}^{\infty}\left(-A_{ij}(\rho)\frac{d}{d\rho}-\frac{d}{d\rho}A_{ij}(\rho)-\frac{A_{ij}(\rho)}{\rho}+H_{ij}(\rho)\right)\chi_j(\rho), \tag{18}$$

where $A = \{A\}_{ij}$ is anti-Hermitian and $H = \{H\}_{ij}$ is the Hermitian matrix,

$$A_{ij}(\rho) = \left\langle B_i(\rho,\theta) \left| \frac{\partial}{\partial\rho} B_j(\rho,\theta) \right.\right\rangle, \; H_{ij}(\rho) = \left\langle \frac{\partial}{\partial\rho} B_i(\rho,\theta) \left| \frac{\partial}{\partial\rho} B_j(\rho,\theta) \right.\right\rangle. \tag{19}$$

The matrix elements $\{A\}_{ij} = -\{A\}_{ji}$, $\{H\}_{ij} = \{H\}_{ji}$ (see Fig. 2) have the following asymptotics for large

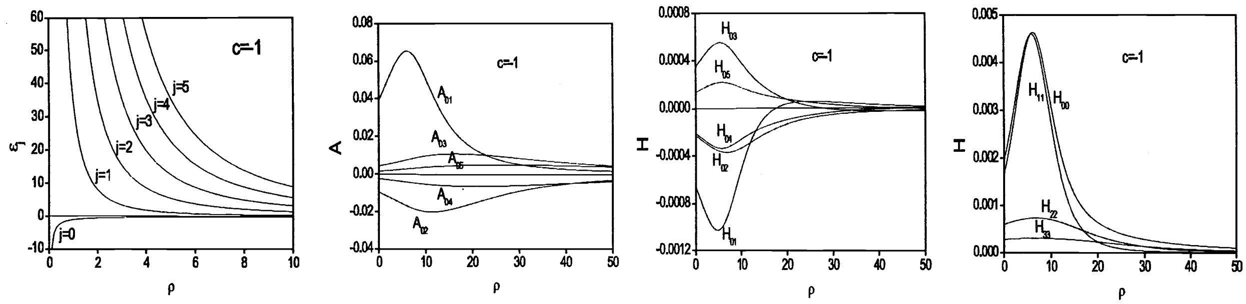

Figure 2: The potential curves $\epsilon_j(\rho)$ and matrix elements $A_{ij}(\rho)$ and $H_{ij}(\rho)$.

and small ρ in the case of finite values of index i and j:

$$\begin{aligned}
\rho \to 0, \quad A_{0j} &= -\frac{(-1)^j\sqrt{2}}{j^2}\left[\frac{1}{36} + \frac{\rho}{j^2}\left(\frac{1}{864} + \frac{\pi^2 j^2}{3888}\right) + \ldots\right], \\
\rho \to 0, \quad A_{ij} &= \frac{(-1)^{i+j}}{i^2 - j^2}\left[\frac{1}{18} + \rho\frac{1}{1296}\left(\frac{1}{i^2} + \frac{1}{j^2}\right) + \ldots\right], \\
\rho \to 0, \quad H_{00} &= \frac{\pi^4}{58320} + \frac{\pi^6}{2204496}\rho + \frac{31\pi^8}{5952139200}\rho^2 + \ldots, \\
\rho \to 0, \quad H_{jj} &= \frac{1}{j^4}\left(-\frac{1}{1728} + \frac{\pi^2 j^2}{3888}\right) + \frac{\rho}{j^6}\left(-\frac{13}{93312} + \frac{\pi^2 j^2}{17496}\right) + \ldots, \\
\rho \to 0, \quad H_{0j} &= \frac{(-1)^j\sqrt{2}}{j^4}\left[\frac{7}{2592} - \frac{\pi^2 j^2}{888} + \frac{\rho}{j^2}\left(\frac{17}{62208} + \frac{1\pi^2 j^2}{139968} - \frac{7\pi^2 j^2}{2099520}\right) + \ldots\right], \\
\rho \to 0, \quad H_{ij} &= \frac{(-1)^{(i+j)}}{(i^2 - j^2)^2}\left[\frac{5}{648} - \frac{1}{1296}\left(\frac{i^2}{j^2} + \frac{j^2}{i^2}\right)\right. \\
&+ \rho\left(-\frac{\pi^2}{11664} + \frac{1}{3456}\left(\frac{1}{i^2} + \frac{1}{j^2}\right) - \frac{11}{93312}\left(\frac{i^2}{j^4} + \frac{j^2}{i^4}\right)\right. \\
&+ \left.\left.\frac{\pi^2}{23328}\left(\frac{i^2}{j^2} + \frac{j^2}{i^2}\right)\right)\right], \\
\rho \to \infty, \quad A_{0j} &= \frac{432(-1)^j(j - 1/2)}{\pi^2\rho^2\sqrt{\rho}} + \frac{23328(-1)^j(j - 1/2)}{\pi^4\rho^3\sqrt{\rho}} + \ldots, \\
\rho \to \infty, \quad A_{ij} &= \frac{(-1)^{(i+j)}(j - 1/2)(i - 1/2)}{(i - 1/2)^2 - (j - 1/2)^2}\left[\frac{72}{\pi^2\rho^2} + \frac{2592}{\pi^4\rho^3}\right. \\
&- \left.\frac{46656}{\pi^6\rho^4}(2 - \pi^2((j - 1/2)^2 + (i - 1/2)^2)) + \ldots\right], \\
\rho \to \infty, \quad H_{00} &= \frac{1}{4\rho^2} + e^{-\frac{\pi^2}{18}\rho}\left(-\frac{\pi^2}{18\rho} - \frac{\pi^4}{324} + \frac{\pi^6}{17496}\rho\right) + \ldots,
\end{aligned}$$

$$\rho \to \infty, \quad H_{jj} = -\frac{108}{\pi^4\rho^4}\left(3+4\pi^2(j-1/2)^2\right) - \frac{7776}{\pi^6\rho^5}\left(3+16\pi^2(j-1/2)^2\right) + ...,$$

$$\rho \to \infty, \quad H_{0j} = \frac{216(-1)^j(j-1/2)}{\pi^2\rho^3\sqrt{\rho}} - \frac{11664(-1)^j(j-1/2)}{\pi^4\rho^4\sqrt{\rho}} + ...,$$

$$\begin{aligned} \rho \to \infty, \quad H_{ij} &= \frac{(-1)^{(i+j)}(i-1/2)(j-1/2)}{(i-j)^2(i+j-1)^2}\left[\frac{5184}{\pi^4\rho^4}\left((j-1/2)^2+(i-1/2)^2\right)\right. \\ &+ \frac{93312}{\pi^6\rho^5}\left(\pi^2\left((i-1/2)^2-(j-1/2)^2\right)^2\right. \\ &\qquad \left.\left.+4\left((i-1/2)^2+(j-1/2)^2\right)\right) + ...\right]. \end{aligned}$$

2.1. Multichannel scattering problem

Let us consider the elastic scattering problem of the third particle on a pair of particles in ground state 0. Let us rewrite (18) separating the ground 0 and the excited j states:

$$\begin{cases} \left(\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho}+q^2\right)\chi_0(\rho)\tilde{V}_0(\rho)\chi(\rho), \\ \left(\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho}-k^2\right)\chi_i(\rho)=\tilde{V}_i(\rho)\chi(\rho), \ i \neq 0. \end{cases} \tag{20}$$

Here $0 \leq q^2 = 2E - \epsilon_0^{(0)} \leq -\epsilon_0^{(0)}$, q is the relative momentum of the third particle counted from a two-particle threshold, $\epsilon_0^{(0)} = -(\pi/6)^2$, $\epsilon_0^{(0)} \leq -k^2 < 0$ is the energy of the system of three particles below the three-partial threshold, and the effective potentials of the ground $\tilde{V}_0(\rho)$ and excited $\tilde{V}_i(\rho)$ states are given by the relations

$$\begin{aligned} \tilde{V}_0(\rho)\chi(\rho) &= \sum_{j=1}^{\infty}\left(-A_{0j}(\rho)\frac{d}{d\rho}-\frac{d}{d\rho}A_{0j}(\rho)-\frac{A_{0j}(\rho)}{\rho}+H_{0j}(\rho)\right)\chi_j(\rho)+(H_{00}(\rho)+\epsilon_0(\rho)-\epsilon_0^{(0)})\chi_0(\rho), \\ \tilde{V}_i(\rho)\chi(\rho) &= \sum_{j=0,i\neq j}^{\infty}\left(-A_{ij}(\rho)\frac{d}{d\rho}-\frac{d}{d\rho}A_{ij}(\rho)-\frac{A_{ij}(\rho)}{\rho}+H_{ij}(\rho)\right)\chi_j(\rho)+(H_{ii}(\rho)+\epsilon_i(\rho))\chi_i(\rho), \ i\neq 0. \end{aligned} \tag{21}$$

The formal solutions of the system (20, 21) can be represented as

$$\begin{cases} \chi_0(\rho) = J_0(q\rho) + \frac{\pi}{2}\int_0^\infty J_0(q\rho_<)Y_0(q\rho_>)\tilde{V}_0(\rho')\chi(\rho')\rho' d\rho', \\ \chi_i(\rho) = -\int_0^\infty K_0(k\rho_>)I_0(k\rho_<)\tilde{V}_i(\rho')\chi(\rho')\rho' d\rho', \ i \neq 0. \end{cases} \tag{22}$$

Here $\rho_> = \max\{\rho, \rho'\}$, $\rho_< = \min\{\rho, \rho'\}$ and $J_i(\rho)$, $Y_i(\rho)$ are the cylindrical Bessel functions of the first and second type, $I_i(\rho)$, $K_i(\rho)$ are the modified cylindrical Bessel functions of the first and second type.

It should be noted that in the second integral equation of the system (22) the function $\tilde{V}_i(\rho)\chi(\rho)\rho$ at $i \neq 0$ at $\rho = 0$ has the singularity $\sim 1/\rho$, which should be taken into account in the definition of the Green function. Thus the system of equations (18) may be rewritten as:

$$\begin{cases} \left(\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho}+q^2\right)\chi_0(\rho)=V_0(\rho)\chi(\rho), \\ \left(\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho}-\left(\frac{6i}{\rho}\right)^2-k^2\right)\chi_i(\rho)=V_i(\rho)\chi(\rho), \ i \neq 0, \end{cases} \tag{23}$$

and the following designations can be introduced:

$$\begin{aligned} V_0(\rho)\chi(\rho) &= \sum_{j=1}^{\infty}\left(-A_{0j}(\rho)\frac{d}{d\rho}-\frac{d}{d\rho}A_{0j}(\rho)-\frac{A_{0j}(\rho)}{\rho}+H_{0j}(\rho)\right)\chi_j(\rho)+(H_{00}(\rho)+\epsilon_0(\rho)-\epsilon_0^{(0)})\chi_0(\rho), \\ V_i(\rho)\chi(\rho) &= \sum_{j=0,i\neq j}^{\infty}\left(-A_{ij}(\rho)\frac{d}{d\rho}-\frac{d}{d\rho}A_{ij}(\rho)-\frac{A_{ij}(\rho)}{\rho}+H_{ij}(\rho)\right)\chi_j(\rho)+(H_{ii}(\rho)+\epsilon_i(\rho)-\left(\frac{6i}{\rho}\right)^2)\chi_i(\rho). \end{aligned} \tag{24}$$

Using the Green function the formal solutions of the system (23, 24) can be represented in integral form

$$\begin{cases} \chi_0(\rho) = J_0(q\rho) + \frac{\pi}{2}\int_0^\infty J_0(q\rho_<)Y_0(q\rho_>)V_0(\rho')\chi(\rho')\rho' d\rho', \\ \chi_i(\rho) = -\int_0^\infty K_{6i}(k\rho_>)I_{6i}(k\rho_<)V_i(\rho')\chi(\rho')\rho' d\rho', \; i \neq 0. \end{cases} \tag{25}$$

As follows from (16) the integrand function $V_i(\rho)\chi(\rho)\rho$ has no peculiarity at the point $\rho = 0$.

The asymptotic of solution $\chi_0(\rho)$ at $\rho \to \infty$ is as follows:

$$\chi_0(\rho)\Big|_{\rho\to\infty} \to J_0(q\rho) + \mu Y_0(q\rho) \to \sqrt{\frac{2}{q\pi\rho}}\left(\sin\left(q\rho + \frac{\pi}{4}\right) - \mu\cos\left(q\rho + \frac{\pi}{4}\right)\right) \tag{26}$$

$$\lambda^{-1} = \frac{2}{\pi}\mu = \frac{2}{\pi}\tan(\delta') = \int_0^\infty J_0(q\rho)V_0(\rho)\chi(\rho)\rho d\rho, \tag{27}$$

$$\delta = \frac{\pi}{4} - \delta' + \pi m \quad m = 0, 1, 2, \dots. \tag{28}$$

Here $\delta = \delta(q)$ is the value of the required phase shift at the fixed value of momentum $0 \leq q \leq \pi/6$. Using the expression (27), obtained as a result of transformation identical to (25), one can gets the following system of integral equations

$$\begin{cases} \chi_0(\rho) - \frac{\pi}{2}\int_0^\infty J_0(q\rho_<)Y_0(q\rho_>)V_0(\rho')\chi(\rho')\rho' d\rho' = \lambda J_0(q\rho)\int_0^\infty J_0(q\rho)V_0(\rho)\chi(\rho)\rho d\rho, \\ \chi_i(\rho) + \int_0^\infty K_{6i}(k\rho_>)I_{6i}(k\rho_<)V_i(\rho')\chi(\rho')\rho' d\rho' = 0, \; i \neq 0. \end{cases} \tag{29}$$

Let us introduce the matrix integral operators

$$C(\rho,\rho')\chi(\rho') = \begin{cases} \chi_0(\rho) - \frac{\pi}{2}\int_0^\infty J_0(q\rho_<)Y_0(q\rho_>)V_0(\rho')\chi(\rho')\rho' d\rho', \\ \chi_i(\rho) + \int_0^\infty K_{6i}(k\rho_>)I_{6i}(k\rho_<)V_i(\rho')\chi(\rho')\rho' d\rho', \; i \neq 0, \end{cases}$$
$$D(\rho,\rho')\chi(\rho') = \begin{cases} J_0(q\rho)\int_0^\infty J_0(q\rho)V_0(\rho)\chi(\rho)\rho d\rho, \\ 0, \; i \neq 0, \end{cases} \tag{30}$$

where $\chi(\rho) = (\chi_0(\rho), \chi_1(\rho), ...)^T$ is the vector-function.

Using the (30) we can get the generalized eigenvalue problem for the system of integral equations (29)

$$(C(\rho,\rho') - \lambda D(\rho,\rho'))\chi(\rho') = 0, \tag{31}$$

with respect to a pair of the unknown variables: the vector-function $\chi(\rho')$ and the spectral parameter $\lambda = \frac{\pi}{2}\cot\delta'$. Let us add the condition of orthogonality to Eq. (31)

$$\begin{gathered} F(\lambda,\chi) = (V(\rho)\chi(\rho), (C(\rho,\rho') - \lambda D(\rho,\rho'))\chi(\rho')) = 0, \\ V(\rho)\chi(\rho) = (V_1(\rho)\chi(\rho), V_2(\rho)\chi(\rho), ...)^T. \end{gathered} \tag{32}$$

From this condition of orthogonality we have the expression for calculating the spectral parameter λ

$$\lambda = \frac{(V(\rho)\chi(\rho), C(\rho,\rho')\chi(\rho'))}{(V(\rho)\chi(\rho), D(\rho,\rho')\chi(\rho'))}, \tag{33}$$

which corresponds to the Schwinger variational functional.[3] Eq. (31) can also be derived using variation of this functional.

2.2. Iteration schemes for the solution of the scattering problem

The discretization on appropriate nodes of grid Ω allows us to reduce problem (31), (33) to generalized algebraic eigenvalue problem

$$(\overline{C} - \tilde{\lambda}\overline{D})\tilde{\chi} = 0, \tag{34}$$

$$F(\tilde{\lambda}, \tilde{\chi}) = (V\tilde{\chi}, (\overline{C} - \tilde{\lambda}\overline{D})\tilde{\chi}) = 0, \tag{35}$$

where $\overline{C}$ and $\overline{D}$ are square matrices of dimensions $(Ngrid \times Ndim) \times (Ngrid \times Ndim)$ and $\tilde{\chi}$ is a vector of dimension $Ngrid \times Ndim$. Here $Ngrid$ is the number of nodes of grid Ω_h, $Ndim$ is the number of equations.

Let us represent the eigenvalue problem (34, 35) in the form of a nonlinear equation

$$\varphi(a, \tilde{\lambda}, \tilde{\chi}) = \begin{pmatrix} (\overline{C} - \tilde{\lambda}\overline{D})\tilde{\chi} \\ F(\tilde{\lambda}, \tilde{\chi}) \end{pmatrix} = 0, \tag{36}$$

with respect to the couple of the unknown variable $z = \{\tilde{\lambda},\ \tilde{\chi}\} \in R \times Y,\ Y \subseteq B$, at the fixed value of parameter $a = k \in R$.

Let us consider the scheme of solution of this nonlinear equation using the Continuous Analogue of Newton's Method which consists in the replacement of the source of nonlinear stationary problem (36) with the evolutionary Cauchy problem[9]:

$$\varphi'(a, z(t))\frac{dz(t)}{dt} = -\varphi(a, z(t)), \tag{37}$$

$$z(0) = z_0. \tag{38}$$

Here t $(0 \le t < \infty)$ is the continuous parameter, trajectory $z(t)$ depends on it, φ' is the Frechet derivative, z_0 is the element in a vicinity of the required solution $z^* = (\lambda^*, y^*)$ to (36). The proof of the convergence of continuous trajectory $z(t)$ at $t \to \infty$ to solution z^* under conditions of continuity φ , φ' and existence of the restricted operator $(\varphi')^{-1}$ in the vicinity z^* is based on existing of the integral of the Cauchy problem (37) - (38)

$$\varphi(a, z(t)) = e^{-t}\varphi(a, z_0). \tag{39}$$

The discrete approximation over argument t of the problem (37) - (38) on the basis of the Eulerian representation reduces it to the solving of a succession of linear problems

$$\begin{aligned} &\varphi'(a, z_k)\Delta z_k = -\varphi(a, z_k), \\ &z_{k+1} = z_k + \tau_k \Delta z_k, \end{aligned} \tag{40}$$

and special choice of parameter τ_k can optimize the rate and stability of the convergence $z_k \to z^*$.[10,11]

For the numerical solution of Eq.(36) the iteration scheme[12] (40) was realized:

$$\begin{cases} v_n = -\tilde{\chi}^{(n)}, \\ (\overline{C} - \tilde{\lambda}_n\overline{D})u_n = \overline{D}\tilde{\chi}^{(n)}, \\ \mu_n = \frac{(V\chi^{(n)},\ \overline{C}\chi^{(n)})}{(V\tilde{\chi}^{(n)},\ \overline{D}\tilde{\chi}^{(n)})} - \tilde{\lambda}_n, \\ \tilde{\chi}^{(n+1)} = \tilde{\chi}^{(n)} + \tau_n(v_n + u_n\mu_n), \\ \tilde{\lambda}_{n+1} = \tilde{\lambda}_n + \tau_n\mu_n, \end{cases} \tag{41}$$

where $n = 0, 1, 2, \ldots;\ \{\tilde{\lambda}_0,\ \tilde{\chi}^{(0)}\}$ is the initial approximation from neighborhood of the required solution. To choose the iterative step τ_n, the formula $\tau_n = \Delta(0)/(\Delta(0) + \Delta(1))^{10}$ was applied, where $\Delta(t)$ is the basis component of residual (41) in C^2. Here uniform grid of nodes was used $\Omega_h = \{\zeta_0 = 10^{-5}, \zeta_{i+1} = \zeta_i + h, \zeta_{Ngrid} = 0.999, h = (\zeta_{Ngrid} - \zeta_0)/Ngrid\}$ that approximate the finite interval $0 \le \zeta = \rho/(1+\rho) \le 1$ at the values of $Ngrid = 840$ and $h \approx 0.001248$.

The numerical results of calculations of the phase shift are presented in Table 1. When the number of equations was increased up to $Ndim = 6$ the results converge to the known analytical values with the accuracy up to $5 \cdot 10^{-3}$. Extrapolating the number $Ndim$, the accuracy $1 \cdot 10^{-3}$ is reached. As follows from Table 1, the values of the phase shift are more exact when momentum q is less for the same number of equations. In figure 3 the eigenfunctions $\chi_j,\ j = 0, ..., 5$ at $q = 0.5$ are shown demonstrating convergence of adiabatic expansion (17).

Table 1. The values of phase shift δ depending on momentum q and the number of equations N. For comparison the value of phase shift at $N = 1$, and the exact phase shift[2] $\delta_{exact} = 3/2\pi - arctg(8\sqrt{3}q/\pi/(1 - q^2/(\pi/6)^2))$ are reduced to four digits. In column ∞ the reduced values δ, obtained by extrapolation by the number of equations are shown.

q\ N	1	2	3	4	5	6	∞	[2]	δ_{exact}
0.002	4.066	4.701	4.704	-	-	-	4.705	4.08	4.703
0.10	4.253	4.277	4.280	4.282	4.283	4.284	4.284	4.25	4.283
0.20	3.869	3.899	3.904	3.907	3.908	3.910	3.911	3.87	3.910
0.30	3.557	3.596	3.604	3.607	3.609	3.610	3.612	3.56	3.611
0.40	3.305	3.353	3.363	3.366	3.368	3.369	3.372	3.30	3.373
0.50	3.097	3.157	3.169	3.172	3.174	3.176	3.179	3.10	3.181

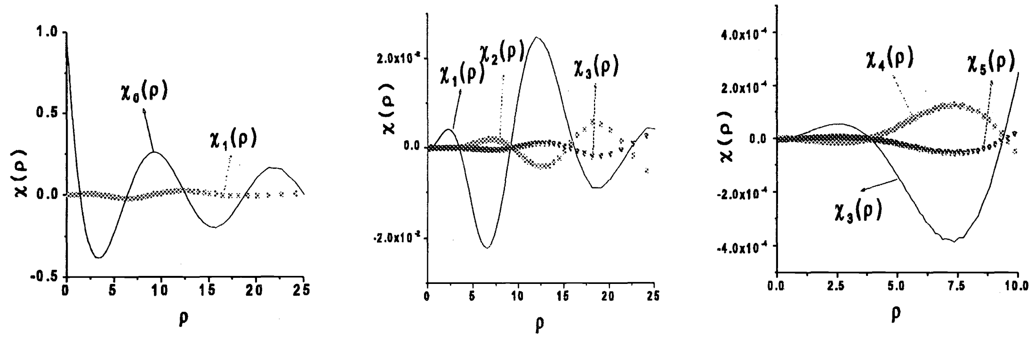

Figure 3: The eigenfunctions $\chi_j(\rho), j = 0, ...5$ of continuous spectrum problem (34, 35) at q=0.5

2.3. The discrete spectrum problem in multichannel approximation

Let us consider the problem of calculation of the bound states of three particles system describing by Eq. (5). In the case of the closed channel 0, the system of equations (18) may be written as follows:

$$\begin{cases} \left(\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho} - q^2\right)\chi_0(\rho) = V_0(\rho)\chi(\rho), \\ \left(\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho} - \left(\frac{6i}{\rho}\right)^2 - k^2\right)\chi_i(\rho) = V_i(\rho)\chi(\rho),\ i \neq 0, \end{cases} \tag{42}$$

where $\varepsilon = q^2(k) = -2E + \epsilon_0^{(0)}$ is the binding energy of the three particle system, measured from the two-particles threshold, $-k^2 = 2E$ is the energy of the three particle system and $V_0(\rho)$ and $V_i(\rho)$ are effective potentials defined by relations (24). Solutions of the system (42) can be presented in the form of integral equations:

$$\begin{cases} \chi_0(\rho) = -\int_0^\infty K_0(q\rho_>)I_0(q\rho_<)V_0(\rho')\chi(\rho')\rho' d\rho', \\ \chi_i(\rho) = -\int_0^\infty K_{6i}(k\rho_>)I_{6i}(k\rho_<)V_i(\rho')\chi(\rho')\rho' d\rho',\ i \neq 0. \end{cases} \tag{43}$$

Let us introduce the matrix integral operators

$$D(\rho,\rho')\chi(\rho') = \begin{cases} -\int_0^\infty K_0(q\rho_>)I_0(q\rho_<)V_0(\rho')\chi(\rho')\rho' d\rho', \\ -\int_0^\infty K_{6i}(k\rho_>)I_{6i}(k\rho_<)V_i(\rho')\chi(\rho')\rho' d\rho',\ i \neq 0. \end{cases} \tag{44}$$

Then (43) become the eigenvalue problem with respect to the vector-functions $\chi(\rho')$ and the spectral parameter k

$$(\mathbf{I} - D(\rho,\rho'))\chi(\rho') = 0, \tag{45}$$

where $\mathbf{I}$ is the unit operator. The eigenfunctions of Eq. (45) should obey to the orthogonality conditions:

$$\begin{aligned} F(k,\chi) &= (V(\rho)\chi(\rho), (\mathbf{I} - D(\rho,\rho'))\chi(\rho')) = 0,\\ V(\rho)\chi(\rho) &= (V_1(\rho)\chi(\rho), V_2(\rho)\chi(\rho), ...)^T. \end{aligned} \tag{46}$$

2.4. Iteration schemes for solving the discrete spectrum problem

The eigenvalue problem (45) and (46) can be presented as nonlinear equation (36)

$$\varphi(k,\chi) = \begin{pmatrix} (\mathbf{I} - D)\chi \\ F(k,\chi) \end{pmatrix} = 0 \tag{47}$$

with respect to $z = \{k,\chi\} \in R\times L_2$ that depend on of the additional parameter $0 \le t < \infty$, i.e.$z(t) = \{k(t),\chi(t)\}$. Then instead of (47) we have the main evolutionary equation for finding the trajectory $z(t)$

$$(\mathbf{I} - D)\frac{d\chi}{dt} - D'_k\chi\frac{dk}{dt} = -(\mathbf{I} - D)\chi \tag{48}$$

with initial conditions $z(0) = \{k(0) = k_0, \chi(0) = \chi^{(0)}\}$ in the vicinity of the required solution, where D'_k is a derivative of the integral operator D for k.

If the operator $V(\mathbf{I} - D)\chi$ is self-conjugate and the condition

$$(\chi, V(\mathbf{I} - D)\chi) = (V\chi, (\mathbf{I} - D)\chi), \tag{49}$$

is fulfilled, then we have the following additional evolutionary equation

$$\left(V\chi, (\mathbf{I} - D)\frac{d\chi}{dt}\right) + \left(V\chi, (\mathbf{I} - D)\frac{d\chi}{dt} - D'_k\frac{dk}{dt}\right) = -(V\chi, (\mathbf{I} - D)\chi), \tag{50}$$

which gives

$$\left(V\chi, (\mathbf{I} - D)\frac{d\chi}{dt}\right) = 0. \tag{51}$$

Using the representation for the total derivative

$$\frac{d\chi}{dt} = \frac{\partial\chi}{\partial t} + \frac{\partial\chi}{\partial k}\frac{dk}{dt}, \tag{52}$$

one can get the system of equations for derivatives

$$\begin{cases} \frac{\partial\chi}{\partial t} = -\chi, \\ (\mathbf{I} - D)\frac{\partial\chi}{\partial k} = D'_k\chi. \end{cases} \tag{53}$$

Substituting (52) in (51) and accounting (53) the expression for the increment can be derived as follows:

$$\frac{dk}{dt} = \frac{(V\chi, (\mathbf{I} - D)\chi)}{(V\chi, D'_k\chi)}. \tag{54}$$

The functional in right-hand side of (54) corresponds to Schwinger variational functional.[3]

Using discretization at the proper grid of nodes Ω_h and approximation (36) of the derivatives of the solution, the problems (45) and (46) are reduced to the algebraic eigenvalue problem

$$(I - \overline{D})\tilde{\chi} = 0, \tag{55}$$

Table 2. The energy of ground state depending on the number of equations N and step h. In last column the reduced value of energy is presented, obtained using the extrapolation according to the step h. $2E = -1.096\,622\,711 + O(1 \cdot 10^{-10}) = -\pi^2/9$.

N	h	h/2	h/4	h→ 0
1	-1.096 514 763	-1.096 460 535	-1.096 447 064	-1.096 442 612
2	-1.096 692 582	-1.096 637 992	-1.096 624 431	-1.096 619 948
3	-1.096 695 093	-1.096 640 489	-1.096 626 924	-1.096 622 440
4	-1.096 695 313	-1.096 640 706	-1.096 627 140	-1.096 622 656
5	-1.096 695 352	-1.096 640 744	-1.096 627 177	-1.096 622 694
6	-1.096 695 362	-1.096 640 755	-1.096 627 178	-1.096 622 705

$$F(\tilde{k}, \tilde{\chi}) = (V\tilde{\chi}, (I - \overline{D})\tilde{\chi}) = 0, \tag{56}$$

where I is the unit matrix. I and $\overline{D}$ are square matrices of dimensions $(Ngrid \times Ndim) \times (Ngrid \times Ndim)$ and $\tilde{\chi}$ is the vector of dimension $Ngrid \times Ndim$. Here $Ngrid$ is the number of nodes of grid Ω_h, and $Ndim$ is the number of equations.

For numerical solution of Eq. (55), the following iteration scheme was used:

$$\begin{cases} v_n = -\tilde{\chi}^{(n)}, \\ (I - \overline{D})u_n = \overline{D}'_k \tilde{\chi}^{(n)}, \\ \mu_n = \dfrac{(V\tilde{\chi}^{(n)},\ (I-\overline{D})\tilde{\chi}^{(n)})}{(V\tilde{\chi}^{(n)},\ \overline{D}'_k\tilde{\chi}^{(n)})}, \\ \tilde{\chi}^{(n+1)} = \tilde{\chi}^{(n)} + \tau_n(v_n + u_n\mu_n), \\ \tilde{k}_{n+1} = \tilde{k}_n + \tau_n\mu_n, \end{cases} \tag{57}$$

where $n = 0, 1, 2, \ldots$; $\{\tilde{k}_0,\ \tilde{\chi}^{(0)}\}$ is the initial approximation from the neighborhood of the required solution. Here uniform grid of nodes was used $\Omega_h = \{\zeta_0 = 10^{-10}, \zeta_{i+1} = \zeta_i + h, \zeta_{Ngrid} = 0.98, h = (\zeta_{Ngrid} - \zeta_0)/Ngrid\}$ that approximates the interval $0 \le \zeta = \rho/(1+\rho) \le 1$ at the values $Ngrid = 200$ and $h \approx 0.0049$.

The results of calculation of the values of energy of the ground state are presented in Table 2. The value of the energy of the ground state obtained using the extrapolation of the results from column $h \to 0$ by the number of equations, coincides with the value of the energy of ground state $2E = -\pi^2/9 = -1.096\,622\,711\ldots$ with accuracy up to 10^{-9}. In figure 4 the eigenfunctions χ_j, $j = 0, \ldots, 5$ are shown demonstrating the convergence of adiabatic expansion (17).

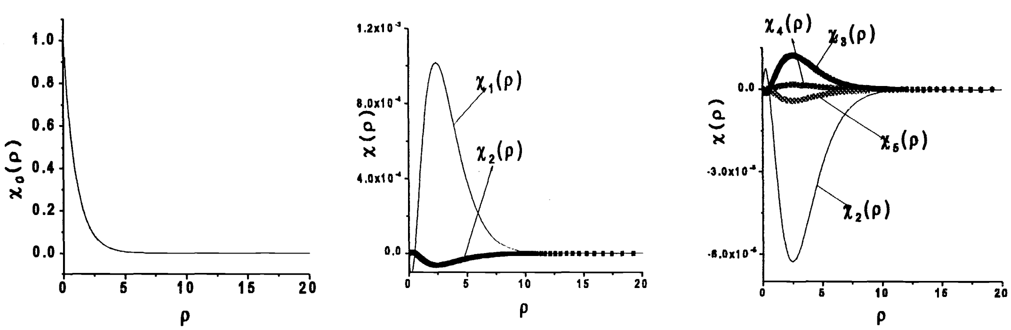

Figure 4: Plots of eigenfunctions $\chi_j(\rho), j = 0, \ldots 5$ of discrete spectrum problem (55, 56).

Remark. At the realization of algorithm (57) to avoid the restriction of computer memory the iterative scheme without inversion of matrix was also used:

$$\begin{cases} (V\tilde{\chi}^{(m)}, \tilde{\chi}^{(m)}) = (V\tilde{\chi}^{(m)}, \overline{D}_{m+1}\tilde{\chi}^{(m)}), \quad \overline{D}_{m+1} = \overline{D}(\tilde{k}_{m+1}) \\ \tilde{\chi}^{(m+1)} = \overline{D}_{m+1}\tilde{\chi}^{(m)}, \; m = 0, 1, 2.... \end{cases} \tag{58}$$

It converges almost 1.5 times slowly than (57).

Conclusion

To solve the scattering problem with a predetermined accuracy, the stable iteration scheme was constructed using the CANM. The multichannel scattering problem was formulated as the eigenvalue problem with respect to the phase shift and the wavefunction using the Schwinger variational functional. The efficiency of proposed iteration scheme was demonstrated using the exact solvable model of elastic scattering of three identical particles (bosons) on a line with pair attractive δ-potentials. The proposed approach allows direct generalization on multi-dimensional and multichannel scattering few-body problems when eligible choice of approximation of solutions is possible, for example, separable potentials, Bateman approximations, as well as trial functions with given variational parameters in the framework of the model of the pair potentials. Beyond of these framework, when asymptotic states with unknown scattering amplitude are given, the parameters of these states can be found using the iteration scheme proposed. The approach under consideration can be extended for solution of problems from nonlinear optics too[13] .

3. ACKNOWLEDGMENT

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