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**LETTER TO THE EDITOR**

# **Three identical particles on a line: comparison of some exact and approximate calculations**

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## **Abstract**

The three-body scattering problem is formulated in the adiabatic representation as a multi-channel spectral problem for a set of coupled one-dimensional integral equations. New stable variational-iteration schemes are developed to calculate the Hamiltonian eigenfunctions and energy eigenvalues, as well as the reaction matrix in the eigenphase shift representation, with prescribed accuracy. The convergence and efficiency of the method are demonstrated in the vicinity of the three-body threshold in the exactly solvable model of three identical particles fixed on a line and coupled with pair-repulsive or attractive zero-range potentials.

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#### **1. Introduction**

Three-particle models with zero-range potentials have found wide applications in atomic physics [1–3]. In particular, such a model was used to describe the weakly bound states and elastic scattering in the system of three helium atoms considered as point particles [2, 3]. In this context it is of great importance to develop approximate methods providing prescribed accuracy, like the conventional variational-iteration approaches [4–6], as well as to test them using appropriate exactly solvable models [7].

In the present letter we consider new stable variational-iteration schemes and apply them to the simplified model of three identical particles on a line with the attractive or repulsive pair delta-function interactions. For this model exact solutions for the three-body S matrix and bound state energy are well known [8–12]. We demonstrate explicitly that this lowdimensional model preserves the most important characteristic features of the three-body problem to be an interesting benchmark for approximate multichannel calculations. Earlier this model was studied in the adiabatic representation mainly analytically to investigate the applicability and capacity of the multichannel adiabatic approach in the scattering problem both below and above the three-body threshold  $3 \rightarrow 3$  [13–17]. Hence, the direct multichannel analysis of the problem under study is a principal question from the viewpoint of both the theoretical and approximate calculations [13, 18].

This letter is organized as follows. In section [2](#page-1-0) we give a brief review of the scattering problem for the exact solvable model of three identical particles fixed on a line with attractive or repulsive delta-function interactions using the one-parametric adiabatic basis that yields a multichannel spectral problem for the set of coupled one-dimensional differential equations. In sections [3–](#page-5-0)[5](#page-9-0) we consider the variational-iteration schemes for solving the spectral problem for the corresponding set of coupled one-dimensional integral equations below and above the three-body scattering threshold  $3 \rightarrow 3$  and examine the efficiency and convergence of our approach. In conclusion we point out briefly the further application of the proposed approach and the model under consideration.

## <span id="page-1-0"></span>**2. The problem of three identical particles in the adiabatic representation**

We consider three identical particles in the centre-of-mass reference frame (CMRF), described by the Jacobi coordinates,  $\eta = 2^{-1/2}(x_1 - x_2), \xi = 6^{-1/2}(x_1 + x_2 - 2x_3)$ , in the plane  $\mathbb{R}^2$ , where  $\{\{x_1, x_2, x_3\} \in \mathbb{R}^3 | x_1 + x_2 + x_3 = 0\}$  are the Cartesian coordinates of the particles on a line. In polar coordinates  $\eta = \rho \cos \theta$ ,  $\xi = \rho \sin \theta$ ,  $-\pi < \theta \leq \pi$ , the Schrödinger equation for the partial wavefunction  $\Psi_i = \Psi_i(\rho, \theta)$  takes the form

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

<span id="page-1-2"></span>Here *E* is the relative energy in the CMRF, *m* is the mass of each particle, the potential function *V*( $\rho$ ,  $\theta$ ) is defined as a sum of identical pair potentials *V*( $\rho$ ,  $\theta$ ) =  $\sum_{l=-1}^{l} V(\sqrt{2}\rho|\cos(\theta - \theta)|)$ *v*(*p*, *v*) is defined as a sum of defined pair potentials *v*(*p*, *v*) =  $\sum_{l=-1}^{n} v (x2p \cos(v - 2l\pi/3))$ . We choose the pair potentials in the form of delta functions  $V(\sqrt{2}\eta) = g\delta(|\eta|)/\sqrt{2}$ of the finite strength  $g = c\bar{\kappa}\sqrt{2}(\hbar^2/m)$ , and consider the case of  $\bar{\kappa} = \pi/6$  [13]. In the case of attraction between the particles *c* = −1 there is a pair bound state  $φ_0(η) = \sqrt{k}$  exp $(-k|η|)$ with the binding energy  $-\epsilon_0^{(0)} = 2E_0^{(0)} = \bar{\kappa}^2$ . Here and below we use the units  $\hbar = m = 1$ . In the case of repulsion  $c = 1$  there are no pair bound states, i.e.  $\epsilon_0^{(0)} = 0$ . Let us decompose the CMRF wavefunction  $\hat{\Psi}$  into the complete orthogonal set of one-parametric adiabatic functions  $B_j \equiv B_j(\rho, \theta)$  and  $B_i^{\text{as}}(\theta') = B_i(\rho \to \infty, \theta')$  [18]

$$
\hat{\Psi} = \sum_{i=0} |\Psi_i\rangle \langle B_i^{\text{as}} | , |\Psi_i\rangle = \sum_{j=0} |B_j\rangle \langle B_j | \Psi_i \rangle = \sum_{j=0} B_j(\rho, \theta) \chi_{ji}(\rho) \tag{2}
$$

<span id="page-1-3"></span>where  $\langle B_j | B_i \rangle = \int_{\Omega} d\theta \bar{B}_j(\rho, \theta) B_i(\rho, \theta) = \delta_{ji}$  is the inner product in the fibres  $H_\rho \sim L_2(\Omega)$ at any fixed  $\rho \in R^1_+$ .

<span id="page-1-1"></span>Following [14], we consider briefly the necessary definitions of the adiabatic functions that satisfy the following differential equation and boundary conditions:

$$
\begin{cases}\n-\frac{1}{\rho^2} \frac{\partial^2 B_j(\rho, \theta)}{\partial \theta^2} = \epsilon_j(\rho) B_j(\rho, \theta) \\
\frac{1}{\rho} \frac{\partial B_j(\rho, \theta)}{\partial \theta}\Big|_{\theta = \pm \frac{\pi}{6} + \frac{\pi \pi}{3}} = \mp \frac{c\pi}{6} B_j(\rho, \theta)\Big|_{\theta = \pm \frac{\pi}{6} + \frac{\pi}{3}}.\n\end{cases}
$$
\n(3)

We also require continuity of the eigenfunctions  $B_j \in W_2^1(\Omega)$  [19]. Such a set, totally symmetric with respect to permutations of particles, and valid for six sectors  $n\pi/3 - \pi/6 \leq$  $\theta < n\pi/3 + \pi/6$ ,  $n = 0, 5$  of the cycle  $\Omega : -\pi < \theta \leq \pi$  is given by

<span id="page-2-1"></span>
$$
B_{j} = \begin{cases} B_{0}^{(C)}(\rho, \theta) = \sqrt{\frac{y_{0}^{2} - x^{2}}{\pi(y_{0}^{2} - x^{2}) - x}} \cosh[6y_{0}\theta_{n}] \\ B_{j}^{(C)}(\rho, \theta) = \sqrt{\frac{y_{j}^{2} + x^{2}}{\pi(y_{j}^{2} + x^{2}) + x}} \cos[6y_{j}\theta_{n}] & j \ge 1 \end{cases} \text{ at } c = -1
$$
  
\n
$$
B_{j} = \begin{cases} B_{j}^{(C)}(\rho, \theta) = \sqrt{\frac{y_{j}^{2} + x^{2}}{\pi(y_{j}^{2} + x^{2}) + x}} \cos[6y_{j}\theta_{n}] & j \ge 0 \\ B_{j}^{(S)}(\rho, \theta) = \sqrt{\frac{y_{j}^{2} + x^{2}}{\pi(y_{j}^{2} + x^{2}) + x}} \sin[6y_{j}\theta_{n}] & j \ge 1 \end{cases} \text{ at } c = 1
$$
\n(4)

where  $x = c \frac{\pi}{36} \rho$  and  $\theta_n = \theta - n\pi/3$ . The eigenvalues  $\epsilon_0(\rho)$  and  $\epsilon_j(\rho)$ ,  $j \ge 1$ , are obtained from the reduced eigenvalues  $y_0(\rho)$  and  $y_j(\rho)$ 

 $\int \frac{f(y_j^2 + x^2) + x}{\pi (y_j^2 + x^2) + x} \sin[6y_j \theta_n]$  *j*  $\geq 1$ 

$$
\epsilon_0(\rho) = c \left(\frac{6y_0(\rho)}{\rho}\right)^2 \qquad \epsilon_j(\rho) = \left(\frac{6y_j(\rho)}{\rho}\right)^2 \tag{5}
$$

which, in turn, are the roots and solutions of the transcendental equations which follow from the boundary conditions [\(3\)](#page-1-1)

$$
\begin{cases}\ny_0^{(C)}(\rho)\tanh(\pi y_0^{(C)}(\rho)) = -x & 0 \le y_0^{(C)}(\rho) > \infty & \text{at } c = -1 \\
y_j^{(C)}(\rho)\tan(\pi y_j^{(C)}(\rho)) = x & j - \frac{1}{2} < y_j^{(C)}(\rho) < j \quad j \ge 1\n\end{cases}
$$
\n
$$
\begin{cases}\ny_j^{(C)}(\rho)\tan(\pi y_j^{(C)}(\rho)) = x & j < y_j^{(C)}(\rho) < j + \frac{1}{2} \quad j \ge 0 \\
y_j^{(S)}(\rho)\cot(\pi y_j^{(S)}(\rho)) = x & j < y_j^{(S)}(\rho) < j + \frac{1}{2} \quad j \ge 1\n\end{cases}
$$
\n(6)

The eigenvalues and eigenfunctions  $\epsilon_j(\rho)$ ,  $B_j(\rho, \theta)$  allow the following expansions for small and large *ρ*:

<span id="page-2-0"></span>
$$
\epsilon_{0}^{(C)}(\rho)|_{\rho \to 0} \to c\frac{1}{\rho} \left(1 - c\frac{\pi^{2}}{108}\rho + \frac{\pi^{4}}{14580}\rho^{2}\right) \qquad B_{0}^{(C)}(\rho, \theta)|_{\rho \to 0} \to \sqrt{\frac{1}{2\pi}}
$$
\n
$$
\epsilon_{j}^{(C)}(\rho)|_{\rho \to 0} \to \left(\frac{6j}{\rho}\right)^{2} \qquad B_{j}^{(C)}(\rho, \theta)|_{\rho \to 0} \to \sqrt{\frac{1}{\pi}} \cos[6j\theta_{n}] \qquad j \geq 1.
$$
\n(7)\n
$$
\epsilon_{j}^{(S)}(\rho)|_{\rho \to 0} \to \left(\frac{6j+3}{\rho}\right)^{2} \qquad B_{j}^{(S)}(\rho, \theta)|_{\rho \to 0} \to \sqrt{\frac{1}{\pi}} \sin[(6j+3)\theta_{n}] \qquad (7)
$$

$$
\epsilon_0^{(C)}(\rho)|_{\rho \to \infty} \to \begin{cases}\n-\frac{\pi^2}{36}(1 + 4 \exp(-\pi^2 \rho/18)) & \text{at } c = -1 \\
\frac{9}{\rho^2} & \text{at } c = 1\n\end{cases}
$$
\n
$$
B_0^{\text{as}}(\theta) = B_0^{(C)}(\rho, \theta)|_{\rho \to \infty} \to \begin{cases}\n\frac{\sqrt{\pi \rho}}{6} \exp(-\rho \pi/6 |\pi/6 - |\theta_n||) & \text{at } c = -1 \\
\sqrt{\frac{1}{\pi}} \cos[3\theta_n] & \text{at } c = 1 \\
\epsilon_j^{(C)}(\rho)|_{\rho \to \infty} \to \left(\frac{6j + 3c}{\rho}\right)^2 & \epsilon_j^{(S)}(\rho)|_{\rho \to \infty} \to \left(\frac{6j}{\rho}\right)^2 \\
\epsilon_j^{(S)}(\rho, \theta)|_{\rho \to \infty} \to \sqrt{\frac{1}{\pi}} \cos[(6j + 3c)\theta_n] \\
B_j^{(S)}(\rho, \theta)|_{\rho \to \infty} \to \sqrt{\frac{1}{\pi}} \sin[6j\theta_n]\n\end{cases}
$$
\n(8)

<span id="page-3-1"></span>Taking the inner product of the elements of the basis  $B_i(\rho, \theta)$  with equation [\(1\)](#page-1-2) and extracting the terms  $\epsilon_i(\rho)$  at small  $\rho$  by equation [\(7\)](#page-2-0), we obtain the set of coupled adiabatic equations

 $\frac{1}{\pi}$  sin[6*j* $\theta_n$ ]

$$
\left(\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\rho\frac{\mathrm{d}}{\mathrm{d}\rho} - \left(\frac{6j}{\rho}\right)^2 + 2E - \epsilon_0^{(0)}\delta_{0j}\right)\chi_{ji}(\rho) = V_{ji}(\rho)\chi_i(\rho). \tag{9}
$$

Here the action of the effective potentials  $V_{ji}(\rho)$  on the eigenvector  $\chi_i(\rho)$  is defined by the relations at fixed number *N* of equations using in approximate calculations

$$
V_{ji}(\rho)\chi_i(\rho) = \sum_{n=0}^{N-1} \left( -A_{jn}(\rho) \frac{d}{d\rho} - \frac{1}{\rho} \frac{d}{d\rho} \rho A_{jn}(\rho) + H_{jn}(\rho) \right) \chi_{ni}(\rho)
$$
  
+ 
$$
\left( \epsilon_j(\rho) - \left( \frac{6j}{\rho} \right)^2 - \epsilon_0^{(0)} \delta_{0j} \right) \chi_{ji}(\rho).
$$
 (10)

Here  $A = \{A\}_{ij}$  is an anti-Hermitian matrix and  $H = \{H\}_{ij}$  is a Hermitian matrix

<span id="page-3-2"></span>
$$
A_{ij}(\rho) = \left\langle B_i(\rho, \theta) \middle| \frac{\partial}{\partial \rho} B_j(\rho, \theta) \right\rangle \qquad H_{ij}(\rho) = \left\langle \frac{\partial}{\partial \rho} B_i(\rho, \theta) \middle| \frac{\partial}{\partial \rho} B_j(\rho, \theta) \right\rangle. \tag{11}
$$

In the case of  $c = 1$  we will use only the set functions  $B^{(C)}$ . Note, we are interested here in the bounded solutions  $\chi_{ji}(\rho)$ , including a vicinity  $\rho \to 0$ . For example, components  $\chi_{j0}$  have behaviour

$$
\chi_{j0}(\rho) = \delta_{j0} + \sum_{l=1}^{6} \chi_{j0,l} \rho^l + O(\rho^7) \qquad \chi_{10,6} \equiv 0 \tag{12}
$$

<span id="page-3-3"></span><span id="page-3-0"></span>where coefficients  $\chi_{j0,l}$  are solutions of an infinite system of the linear algebraic equations that are generated by substitution of [\(12\)](#page-3-0) in equation [\(9\)](#page-3-1). Note, for the truncated system  $\chi_{i0,l}$ are constants except  $\chi_{10,6} \sim \ln \rho$  [17]. For the bound state  $(c = -1)$  the asymptotic form of the solutions at large *ρ* is

$$
\chi_{00}^{\rm as}(\rho) \to C_0 \frac{\mathrm{e}^{-\bar{q}\rho}}{\sqrt{\rho}} \qquad \chi_{j0}^{\rm as}(\rho) \to C_j \frac{\mathrm{e}^{-k\rho}}{\sqrt{\rho}}
$$
(13)

where  $-\epsilon = \bar{q}^2 = -q^2 = -2E + \epsilon_0^{(0)} \ge 0$  is the binding energy of the three-body systems,  $-2E = k^2 > 0$  and  $C_j$  are unknown constants.

For the one-opened-channel scattering problem  $(c = -1)$ , we investigated the asymptotic behaviour of the states both in Jacobi  $[17]$  and polar coordinates [13]. In the representation of standing waves of the open channel  $\epsilon_0^{(0)} < 2E(q) \le 0$  and  $q^2 = 2E - \epsilon_0^{(0)}$ , i.e. at  $0 < q \le \bar{\kappa}$ the asymptotic behaviour at large *ρ* is given by

<span id="page-4-3"></span>
$$
\chi_{00}^{\text{as}}(\rho) \to (J_{1/2}(q\rho) - \tan \delta Y_{1/2}(q\rho)) = \sqrt{\frac{2}{\pi q\rho}} (\sin(q\rho) + \tan \delta \cos(q\rho))
$$
\n(14)

$$
\chi_{j0}^{as}(\rho) \to (\epsilon_j(\rho) - \epsilon_0(\rho))^{-1} \left( A_{j0}(\rho) \frac{d}{d\rho} + \frac{1}{\rho} \frac{d}{d\rho} \rho A_{j0}(\rho) - H_{j0}(\rho) \right) \chi_{00}^{as}(\rho)
$$

where  $\delta = \delta(q)$  is the phase shift,  $J_n(\rho)$  and  $Y_n(\rho)$  are Bessel and Neumann functions [20].

The order of these functions is a consequence of the factor  $1/(4\rho^2)$  which appears in *H*<sub>00</sub>( $\rho$ ) at large  $\rho$  [17]. In this representation the asymptotic wavefunction  $\hat{\Psi}_{0,c=-1}^{as}$  describing the processes below the three-body threshold is defined by the relation [18]

$$
\Psi_{0,c=-1}^{\text{as}} = \Psi_{2\to 2}^{\text{as}} = B_0^{\text{as}} \chi_{00}^{\text{as}} + \sum_{j=1} B_j^{\text{as}} \chi_{j0}^{\text{as}} \tag{15}
$$

where  $\Psi_{2\rightarrow 2}^{as}$  accounts for the conventional  $2 \rightarrow 2$  processes with closed channels.

As follows from the asymptotic expressions for effective potentials [\(11\)](#page-3-2) from [16], for the multi-channel scattering problem the asymptotic behaviour of the solutions  $\chi_{ii}(\rho)$  of equations [\(9\)](#page-3-1) is compatible with the asymptotic boundary conditions above the three-body threshold  $2E = k^2 > 0$ 

$$
\begin{cases}\n\chi_{0i}^{\text{as}}(\rho) \to (-Y_{1/2}(q\rho)\delta_{0i} + J_{1/2}(q\rho)W_{0i}) \\
\chi_{ji}^{\text{as}}(\rho) \to (J_{6j-3}(k\rho)\delta_{ji} + Y_{6j-3}(k\rho)W_{ji})\n\end{cases}
$$
 at  $c = -1$   
\n
$$
\chi_{ji}^{\text{as}}(\rho) \to (J_{6j+3}(k\rho)\delta_{ji} + Y_{6j+3}(k\rho)W_{ji})\n\qquad \text{at } c = 1
$$
\n(16)

<span id="page-4-0"></span>where  $q \geq \bar{\kappa}$ . In this case the eigenphase shifts  $\delta_i$  are calculated via the eigenvalues  $\Lambda$  of the reaction matrix  $(R = {R}j_i)$ , which is related to the *S*-matrix  $(S = {S}j_i)$ 

<span id="page-4-1"></span> $RC = C \Lambda$   $\Lambda = \text{diag}(\tan \delta_0, \tan \delta_1, \ldots)$   $R = \text{i}(I - S)(I + S)^{-1}$ . *.* (17) Here  $C = \{C\}_{ji}$  is the matrix of eigenvectors, and R is the matrix expressed as  $R = \{W\}_{ji}^{-1}$ via the inverse matrix *W* from [\(16\)](#page-4-0).

The asymptotic wavefunctions  $\hat{\Psi}^{as}$  describing the processes above the three-body threshold in cases of attraction  $c = -1$  and repulsion  $c = 1$  are defined by [18]

$$
\begin{cases}\n\hat{\Psi}_{c=-1}^{\text{as}} = \hat{\Psi}_{-}^{\text{as}} + \hat{\Psi}_{+}^{\text{as}},\\ \n\hat{\Psi}_{-}^{\text{as}} = \hat{\Psi}_{2 \to 2}^{\text{as}} + \hat{\Psi}_{2 \to 3}^{\text{as}} = B_{0}^{\text{as}} \chi_{00}^{\text{as}} \bar{B}_{0}^{\text{as}} + \sum_{j=1} B_{j}^{\text{as}} \chi_{j0}^{\text{as}} \bar{B}_{0}^{\text{as}},\\ \n\hat{\Psi}_{+}^{\text{as}} = \hat{\Psi}_{3 \to 2}^{\text{as}} + \hat{\Psi}_{3 \to 3}^{\text{as}} = \sum_{i=1} B_{0}^{\text{as}} \chi_{0i}^{\text{as}} \bar{B}_{i}^{\text{as}} + \sum_{i=1} \sum_{j=1} B_{j}^{\text{as}} \chi_{ji}^{\text{as}} \bar{B}_{i}^{\text{as}},\\ \n\hat{\Psi}_{c=1}^{\text{as}} = \hat{\Psi}_{3 \to 3}^{\text{as}} = \sum_{i=0} \sum_{j=0} B_{j}^{\text{as}} \chi_{ji}^{\text{as}} \bar{B}_{i}^{\text{as}},\n\end{cases} (18)
$$

where  $\Psi_{2\rightarrow 2}^{as} = \langle \hat{\Psi}_{2\rightarrow 2}^{as} | B_0^{as} \rangle$ ,  $\Psi_{2\rightarrow 3}^{as} = \langle \hat{\Psi}_{2\rightarrow 3}^{as} | B_0^{as} \rangle$ ,  $\hat{\Psi}_{3\rightarrow 2}^{as}$  and  $\hat{\Psi}_{3\rightarrow 3}^{as}$  account for the conventional  $2 \rightarrow 2$ , breakup  $2 \rightarrow 3$ , recombination  $3 \rightarrow 2$  and to  $3 \rightarrow 3$  processes, respectively.

<span id="page-4-2"></span>Conventionally the elements of the *S*-matrix for transitions  $3 \rightarrow 3$  are determined by

$$
S_{ji}(k) = -6 \int_{-\pi/6}^{\pi/6} d\theta \int_{-\pi/6}^{\pi/6} d\theta' \bar{B}_{j}^{as}(\theta) \hat{S}_{33}(-\theta, \theta', k) B_{i}^{as}(\theta'). \tag{19}
$$

Here  $\hat{S}_{33}(\theta, \theta', k) = -6 \sum_{i,j} B_j^{as}(-\theta) S_{ji}(k) \bar{B}_i^{as}(\theta')$  is the kernel of the operator  $\hat{S}_{33}$ , which turns the amplitude of the incoming spherical wave in  $\mathbb{R}^2$  into that of the outgoing spherical wave, and the subscripts *i*, *j* run 0, 1, ... at  $c = 1$  and 1, 2, ... at  $c = -1$ . Then the exact matrix elements  $S_{ii}^{\text{exact}}(k)$ , needed for comparison with the numerical results  $S_{ii}(k)$  from [\(17\)](#page-4-1), can be calculated via [\(19\)](#page-4-2) using the known analytical expression [15]

$$
\hat{S}_{33}^{\text{exact}}(\theta, \theta', k) = P(\pi/3 - \theta, k)P(\theta, k)P(\pi/3 + \theta, k)\delta(\theta - \theta')
$$
 (20)

where  $P(\theta, k) = (\mathrm{i}k \cos(\theta) + c\bar{k})/(\mathrm{i}k \cos(\theta) - c\bar{k})$ .

In the case of  $c = -1$  under consideration the processes  $2 \rightarrow 3$  and  $3 \rightarrow 2$  are forbidden, i.e. the matrix elements  $S_{j0}^{\text{exact}} = S_{0j}^{\text{exact}} \equiv 0$ , while the matrix element  $S_{00}^{\text{exact}}$  of the *S*-matrix for the  $2 \rightarrow 2$  process is determined by the relations [15, 17]

<span id="page-5-3"></span>
$$
S_{00}^{\text{exact}}(q) = -P\left(\frac{\pi}{3} - \gamma(\sqrt{2E}), \sqrt{2E}\right) P(\gamma(\sqrt{2E}), \sqrt{2E}) = e^{i\pi} \frac{q + iq_1}{q - iq_1} \frac{q + iq_0}{q - iq_0}.
$$
 (21)

Here  $\gamma(\sqrt{2E})$  satisfies the equation  $i\sqrt{2E}\cos(\pi/3 + \gamma(\sqrt{2E})) = -\bar{\kappa}, q_0 = \pi/(2$ √ 3*)* and *Here*  $\gamma(\sqrt{2}E)$  satisfies the equation  $1\sqrt{2}E \cos(\pi/3 + \gamma(\sqrt{2}E)) = -\kappa$ ,  $q_0 = \pi/(\sqrt{2}\sqrt{3})$  and  $q_1 = \pi/6\sqrt{3}$ ). Then the values of the exact phase shift  $\delta_{\text{exact}} = \delta_{\text{exact}}(q)$ , needed for the comparison with the numerical ones  $\delta$  from [\(14\)](#page-4-3), read as  $\delta_{\text{exact}}(q) = \pi + (2i)^{-1} \ln S_{00}^{\text{exact}}(q)$ . Note that  $-\epsilon_{\text{exact}} = q_0^2 = -\pi^2/36 + \pi^2/9 = \pi^2/12$  is the exact binding energy of the three-body ground state counted off the pair threshold to compare with the numerical one  $\epsilon$ from [\(13\)](#page-3-3).

# <span id="page-5-0"></span>**3. The bound state problem in the multichannel approximation**

<span id="page-5-1"></span>Let us consider the problem of calculating the bound states of the three-body system at  $c = -1$ . In this case the solutions of equations [\(9\)](#page-3-1) can be represented by the integral equations

$$
(\mathbf{I} - D(\rho, \rho')) \chi(\rho') = 0. \tag{22}
$$

Here **I** is a unit operator and  $D(\rho, \rho')$  is the matrix integral operator defined by the following relations

$$
D(\rho, \rho')\chi(\rho') = -\int_0^\infty K_{6j}(t\rho_>) I_{6j}(t\rho_<) V_{j0}(\rho')\chi_0(\rho')\rho' d\rho' \qquad j = \overline{0, N-1} \qquad (23)
$$

where  $t = \bar{q}$  at  $j = 0$ ,  $t = k$  at  $j \neq 0$ ,  $\rho > \frac{1}{2}$  max{ $\rho$ ,  $\rho'$ },  $\rho < \frac{1}{2}$  min{ $\rho$ ,  $\rho'$ } and  $I_j(\rho)$ ,  $K_i(\rho)$  are the modified cylindrical Bessel functions of the first and second kinds [20]. The eigenfunctions of equation [\(22\)](#page-5-1) satisfy the condition of orthogonality of the Schwinger type

$$
F(k, \chi) = (V(\rho)\chi(\rho), (I - D(\rho, \rho'))\chi(\rho')) = 0
$$
\n(24)

where  $V(\rho)\chi(\rho) = (V_{00}(\rho)\chi_0(\rho), V_{10}(\rho)\chi_0(\rho), \ldots)^T$ . Making use of the finite-difference approximation of the derivatives on a properly chosen grid with nodes  $\Omega_h$ , we come to the algebraic eigenvalue problem

$$
(I - \overline{D})\tilde{\chi} = 0 \qquad F(\tilde{k}, \tilde{\chi}) = (V\tilde{\chi}, (I - \overline{D})\tilde{\chi}) = 0 \tag{25}
$$

<span id="page-5-2"></span>where *I* is the unit matrix; *I* and  $\overline{D}$  are square matrices having the dimensions  $(M \times N) \times$  $(M \times N)$  and  $\tilde{\chi}$  is a vector having the dimension  $M \times N$ . Here *M* is the number of nodes of

<span id="page-6-1"></span>**Table 1.** A comparison of the convergence rate of expansion [\(2\)](#page-1-3) with parametric functions  $B(\rho, \theta)$ and free functions  $B(\rho, \theta)|_{\rho \to 0}$  for the differences  $\Delta E = -2E^h + 2E^{\text{exact}}$  of the calculated energy values  $2E^h$  and an exact energy  $2E^{\text{exact}} = -\pi^2/9$  of the three-body ground state versus the number *N* of equations [\(9\)](#page-3-1). The first column shows the number of equations *N*, the second one displays the accuracy of calculations with the parametric functions [\(4\)](#page-2-1) and the last column shows the convergence with the free functions [\(7\)](#page-2-0). Here factor *x* in brackets means  $(x) \equiv 10^x$ .

N	ΛE	ΛE
-1	$1.801(-04)$	$9.662(-2)$
$\mathcal{L}$	$2.762(-06)$	$4.116(-2)$
3	$2.697(-07)$	$2.573(-2)$
4	$5.413(-08)$	$1.866(-2)$
5	$1.594(-08)$	$1.462(-2)$
6	$5.950(-09)$	$1,201(-2)$

<span id="page-6-0"></span>the grid  $\Omega_h$  and N is the number of equations. Numerical solution of equation [\(25\)](#page-5-2) was carried out using the Newtonian iteration scheme with respect to  $v_n$ ,  $u_n$ ,  $\mu_n$ , considered as unknowns:

$$
\begin{cases}\nv_n = -\tilde{\chi}^{(n)} \\
(I - \overline{D})u_n = \overline{D}'_k \tilde{\chi}^{(n)} \\
\mu_n = \frac{(V\tilde{\chi}^{(n)}, (I - \overline{D})\tilde{\chi}^{(n)})}{(V\tilde{\chi}^{(n)}, \overline{D}'_k \tilde{\chi}^{(n)})} \\
\tilde{\chi}^{(n+1)} = \tilde{\chi}^{(n)} + \tau_n(v_n + u_n \mu_n) \\
\tilde{k}_{n+1} = \tilde{k}_n + \tau_n \mu_n\n\end{cases}
$$
\n(26)

where  $n = 0, 1, 2, \ldots$ ; { $\tilde{k}_0, \tilde{\chi}^{(0)}$ } is the initial approximation of the required solution. Here the uniform grid is used  $\Omega_h = \{\zeta_0 = 10^{-10}, \zeta_{i+1} = \zeta_i + h, \zeta_M = 0.98, h = (\zeta_M - \zeta_0)/M\}$ that approximates the finite interval  $0 \le \zeta = \rho/(1+\rho) \le 1$  at the value  $M = 200$  and  $h \approx 0.005$ . The iterative step  $\tau_n$  is chosen to be expressed as  $\tau_n = \Delta_n(0)/(\Delta_n(0) + \Delta_n(1))$ to provide the minimization of the residual  $\Delta_n = ||(I - \overline{D})u_n|| \in C^2$  of equations [\(26\)](#page-6-0) following [6]. The iterations are stopped when the residual equals the prescribed accuracy 10<sup>−</sup>12. The results of our calculations of the energy 2*E<sup>h</sup>* of the three-body ground state (b) are presented in table [1,](#page-6-1) as a difference  $\Delta E = -2E^h + 2E^{\text{exact}}$  with respect to the exact value  $2E^{\text{exact}} = -\pi^2/9$ . For comparison we also display in the last column the results of calculations using expansion [\(2\)](#page-1-3) with the free functions  $B(\rho, \theta)|_{\rho \to 0}$  defined by [\(7\)](#page-2-0). One can see that in the attractive case  $c = -1$  a convergence takes place only for expansion [\(2\)](#page-1-3) with the parametric functions [\(4\)](#page-2-1).

From the approximation using only one equation and only the eigenpotential (without  $H_{00}$ ), we conclude that there is an additional three-body bound state [17]. This is a very weakly bound state, and in this approximation it provides an estimate of the lower bound of the energy. Adding  $H_{00}$  yields the upper bound and eliminates this state. Hence, using the first equation  $(N = 1)$  of the set [\(22\)](#page-5-1) with the potential  $V_0^{BO}(\rho) = \epsilon_0(\rho) - \epsilon_0^{(0)}$ , we reproduce the old lower bound (Born–Oppenheimer or extreme adiabatic) estimate  $2E^{BO} \approx -0.275113 = -\pi^2/36 - 0.00096$ , that corresponds to the phase shift  $\delta_{BO} = 2\pi$ at  $q = 0$  [17]. Solving the set [\(22\)](#page-5-1) of six coupled equations ( $N = 6$ ) in the grid of nodes  $\Omega_h$  at  $\rho_{\text{max}} = 60$  by means of [\(26\)](#page-6-0), we obtained the new upper bound estimate  $2E_{hb}^{N=6} = -0.2739$  for the energy of this state. This is to be compared to  $-\pi^2/36$  which equals  $-0.274155$ . Thus, we have a value very slightly above the exact value  $-\pi^2/36$  that corresponds to zero binding and is associated with the correct phase shift behaviour of 3*π/*2

as *q* tends to zero. We call the state 'half-bound' (hb) and display the calculated solution in the conclusion.

#### **4. The elastic scattering problem with closed channels**

<span id="page-7-1"></span>Let us consider the problem of elastic scattering of the third particle on the pair of other particles below the three-body threshold at  $c = -1$ . Using the Green function corresponding to the left-hand side of equations [\(9\)](#page-3-1), it can be presented in the integral form

$$
\chi_{j0}(\rho) = J_0(q\rho)\delta_{0j} - \int_0^\infty G_j(t,\rho,\rho')V_{j0}(\rho')\chi_0(\rho')\rho' d\rho'
$$
 (27)

where  $G_0(t, \rho, \rho') = -\frac{\pi}{2} J_0(q\rho_<) Y_0(q\rho_<)$  and  $G_j(t, \rho, \rho') = K_{6j}(k\rho_>) I_{6j}(k\rho_<)$ ,  $j \ge 1$ . The integrand  $V_{j0}(\rho)\chi_0(\rho)\rho$  has no singularity at the point  $\rho = 0$ , and the asymptotic form of the solution  $\chi_{00}(\rho)$ , as  $\rho \to \infty$ , is  $\chi_{00}(\rho)|_{\rho \to \infty} \to J_0(q\rho) - \tan \delta' Y_0(q\rho)$ , where  $\tan \delta'$  is determined by the relation

$$
\lambda = -\frac{\pi}{2} \cot \delta' \qquad \lambda^{-1} = \int_0^\infty J_0(q\rho) V_{00}(\rho) \chi_0(\rho) \rho \, d\rho. \tag{28}
$$

<span id="page-7-0"></span>The phase shift  $\delta = \delta(q)$  at the fixed value of the momentum  $0 < q \leq \pi/6$ , according to the definition [\(14\)](#page-4-3), can then be expressed in terms of  $\delta' = \delta'(q)$  as  $\delta = \frac{\pi}{4} + \delta' + \pi$ . Thus, in the  $V_{00}$  mentioned above we have a long-range centrifugal force, which does not follow from the interaction that yields equation [\(14\)](#page-4-3). The relationship between  $J_{1/2}$  and  $J_0$ yields asymptotically the difference in the phase shift equal to  $\pi/4$ . Using expression [\(28\)](#page-7-0) and equations [\(27\)](#page-7-1), we arrive at the generalized eigenvalue problem for the set of integral equations with respect to a pair of unknown variables, namely, the vector function  $\chi_0(\rho')$  and the spectral parameter *λ*:

$$
(C(\rho, \rho') - \lambda D(\rho, \rho')) \chi(\rho') = 0.
$$
\n
$$
(29)
$$

<span id="page-7-2"></span>Here the matrix integrals  $C(\rho, \rho')$  and  $D(\rho, \rho')$  are operators defined by the relations

$$
C(\rho, \rho')\chi(\rho') = \chi_{j0}(\rho) + \int_0^\infty G_j(t, \rho, \rho')V_{j0}(\rho')\chi_0(\rho')\rho'd\rho'
$$
  
\n
$$
D(\rho, \rho')\chi(\rho') = \delta_{0j}J_0(q\rho)\int_0^\infty J_0(q\rho)V_{00}(\rho)\chi_0(\rho)\rho
$$
  
\n
$$
j = \overline{0, N - 1}.
$$
 (30)

<span id="page-7-3"></span>Let us add the Schwinger-type condition of orthogonality to equation [\(29\)](#page-7-2)

$$
F(\lambda, \chi) = (V(\rho)\chi(\rho), (C(\rho, \rho') - \lambda D(\rho, \rho'))\chi(\rho')) = 0
$$
\n(31)

where  $V(\rho)\chi(\rho) = (V_{00}(\rho)\chi_0(\rho), V_{10}(\rho)\chi_0(\rho), ...)$ <sup>T</sup>. In this case if  $k = 0$ , or in the threshold case  $q = \pi/6$ , instead of [\(27\)](#page-7-1) it is necessary to use the following equation

$$
\chi_{j0}(\rho) = -\frac{1}{12j} \int_0^\infty \rho^{6j}_{\leq} \rho^{-6j}_{>} V_{j0}(\rho') \chi_0(\rho') \rho' d\rho' \quad \text{at} \quad j \geq 1. \tag{32}
$$

<span id="page-7-4"></span>After discretization on the grid with the nodes  $\Omega$  the solution of equations [\(29\)](#page-7-2) and [\(31\)](#page-7-3) is reduced to the generalized algebraic eigenvalue problem

$$
(\overline{C} - \tilde{\lambda}\overline{D})\tilde{\chi} = 0 \qquad F(\tilde{\lambda}, \tilde{\chi}) = (V\tilde{\chi}, (\overline{C} - \tilde{\lambda}\overline{D})\tilde{\chi}) = 0 \tag{33}
$$

where  $\overline{C}$  and  $\overline{D}$  are square matrices with the dimensions  $(M \times N) \times (M \times N)$ , and  $\tilde{\chi}$  is a vector with the dimension  $M \times N$ . Here *M* is the number of nodes of the grid  $\Omega_h$ , *N* is the number of equations forming the set [\(29\)](#page-7-2).

<span id="page-8-1"></span>**Table 2.** Values of the phase shift *δ* depending on the momentum *q* and the number of equations *N*. For comparison, the values of the phase shift  $\delta_{\text{BO}} = \delta - \pi/4$  calculated from the first equation of the set [\(27\)](#page-7-1) at  $N = 1$  with the potential  $V_0^{BO}(\rho) = \epsilon_0(\rho) - \epsilon_0^{(0)}$  are given in the second column, and the values of the exact phase shift *δ*exact obtained by means of equation [\(21\)](#page-5-3) are listed to four significant digits in the ninth column.

			N					
q	$\delta_{\rm BO}$	1	2	3	4	5	6	$\delta_{\rm exact}$
0.002	5.750	4.086	4.674	4.698	4.702	4.703	4.703	4.704
0.10	3.760	4.253	4.277	4.280	4.281	4.282	4.282	4.283
0.20	3.220	3.871	3.900	3.905	3.907	3.908	3.908	3.911
0.30	2.863	3.558	3.596	3.602	3.605	3.607	3.607	3.611
0.40	2.589	3.305	3.353	3.362	3.365	3.367	3.368	3.373
0.50	2.358	3.096	3.156	3.167	3.171	3.174	3.175	3.182
$\pi/6$	2.322	3.052	3.114	3.126	3.130	3.133	3.134	3.141

<span id="page-8-0"></span>For the numerical solution of equation [\(33\)](#page-7-4) the Newtonian iteration scheme elaborated in [6] has been implemented with respect to the unknowns  $v_n$ ,  $u_n$ ,  $\mu_n$ 

$$
\begin{cases}\nv_n = -\tilde{\chi}^{(n)} \\
(\overline{C} - \tilde{\lambda}_n \overline{D})u_n = \overline{D}\tilde{\chi}^{(n)} \\
\mu_n = \frac{(V\chi^{(n)}, \overline{C}\chi^{(n)})}{(V\tilde{\chi}^{(n)}, \overline{D}\tilde{\chi}^{(n)})} - \tilde{\lambda}_n \\
\tilde{\chi}^{(n+1)} = \tilde{\chi}^{(n)} + \tau_n(v_n + u_n \mu_n) \\
\tilde{\lambda}_{n+1} = \tilde{\lambda}_n + \tau_n \mu_n\n\end{cases} \tag{34}
$$

where  $n = 0, 1, 2, \ldots$ ; { $\tilde{\lambda}_0$ ,  $\tilde{\chi}^{(0)}$ } is the initial approximation taken in the neighbourhood of the required solution. Here a uniform grid of nodes is used  $\Omega_h = {\zeta_0 = 10^{-5}, \zeta_{i+1} = \zeta_i + h}$ ,  $\zeta_M = 0.99$ ,  $h = (\zeta_M - \zeta_0)/M$ , that approximates the finite interval  $0 \le \zeta = \rho/(1 + \rho) \le 1$ at the values of  $M = 840$  and  $h \approx 0.00125$ . At each step of the iteration scheme [\(34\)](#page-8-0) the value of  $\tilde{\lambda}_n$  in the interval [0*, ζ<sub>M</sub>*] is improved by adding the asymptotic correction  $\tilde{\lambda}_n^{\text{as}}$ , calculated according to [\(28\)](#page-7-0) in the interval [ $\zeta_M$ , 1], using the asymptotic solution of equation [\(27\)](#page-7-1). Note that we use the same rule to choose the iterative step  $\tau_n$  as in the previous section. The iterations were stopped if the residual equaled the predetermined accuracy of 10<sup>−</sup>6. It means that the stationary point of the Schwinger functional in the form of  $\mu_n$  defined by [\(34\)](#page-8-0) is achieved. The numerical results for the phase shift are presented in table [2,](#page-8-1) and with the number of equations increasing up to  $N = 6$ , they converge to the known analytic values of the exact phase shift [\(21\)](#page-5-3) [15, 17] with the accuracy of  $1 \times 10^{-3}$ to 6  $\times$  10<sup>-3</sup>. From table [2](#page-8-1) one can see that for the fixed number of equations the values of the phase shift obtained are closer to the exact ones at small momenta. To reach higher accuracy in the calculations of the phase shifts  $\delta$  it is necessary to extend the value  $q\rho_{\text{max}}$  to values greater than 100, or to use asymptotic expansions of the solutions for  $\chi_{j0}(\rho)$ , up to  $O(\rho^{-3/2})$  [13], taking into account the known asymptotic behaviour of the matrix elements *H<sub>jj</sub>*( $\rho$ ). For comparison, the values of the phase shift  $\delta_{BO} = \delta - \pi/4$  found from the first of equations [\(27\)](#page-7-1) with the potential  $V_0^{BO}(\rho) = \epsilon_0(\rho) - \epsilon_0^{(0)}$  at  $N = 1$  are given in the second column.

## <span id="page-9-0"></span>**5. The elastic scattering problem with open channels**

<span id="page-9-2"></span>Let us consider the elastic scattering problem of a third particle on a pair of particles above the three-body threshold. By means of the Green function corresponding to the left-hand side of equations [\(9\)](#page-3-1) it can be represented in the integral form

$$
\chi_{ji}(\rho) = J_{6j}(t\rho)\delta_{ji} + \frac{\pi}{2} \int_0^\infty J_{6j}(t\rho_<) Y_{6j}(t\rho_>) V_{ji}(\rho') \chi_i(\rho') \rho' d\rho'.
$$
 (35)

<span id="page-9-1"></span>Here  $t = k$  at  $j \ge 0$  for  $c = 1$  and  $t = q$  at  $j = 0$ ,  $t = k$  at  $j \ge 1$  for  $c = -1$ . The asymptotic form of the solution  $\chi_{ji}(\rho)$  at  $\rho \to \infty$  is  $\chi_{ji}(\rho)|_{\rho \to \infty} \to J_{6j}(t\rho)\delta_{ji} - Y_{6j}(t\rho)R_{ji}$ , where the mixed parameter  $R_{ji}$  is determined by the relation

$$
-R_{ji} = \frac{\pi}{2} \int_0^\infty J_{6j}(t\rho) V_{ji}(\rho) \chi_i(\rho) \rho \, d\rho.
$$
 (36)

<span id="page-9-3"></span>Using the expression [\(36\)](#page-9-1) and equations [\(35\)](#page-9-2), we arrive at the generalized eigenvalue problem for the system of integral equations with respect to a pair of unknown variables, namely the vector function  $\chi_{ji}(\rho')$  and the spectral parameter  $\lambda_i = -\frac{\pi}{2} R_{ii}^{-1}$ :

$$
(C_i(\rho, \rho') - \lambda_i D_i(\rho, \rho')) \chi_i(\rho') = 0.
$$
\n(37)

Here the matrix integrals  $C_i(\rho, \rho')$  and  $D_i(\rho, \rho')$  are operators defined by the relations

$$
C_{i}(\rho, \rho')\chi_{i}(\rho') = \chi_{ji}(\rho) - \frac{\pi}{2} \int_{0}^{\infty} J_{6j}(t\rho_{<}) Y_{6j}(t\rho_{>}) V_{ji}(\rho')\chi_{i}(\rho')\rho' d\rho'
$$
  
\n
$$
J_{i}(\rho, \rho')\chi_{i}(\rho') = J_{6j}(t\rho)\delta_{ji} \int_{0}^{\infty} J_{6j}(t\rho) V_{ji}(\rho)\chi_{i}(\rho)\rho d\rho
$$
 (38)

<span id="page-9-4"></span>and  $\chi_i(\rho) = (\chi_{0i}(\rho), \chi_{1i}(\rho), \ldots)^T$  is a vector function. Let us add the condition of orthogonality to equation [\(37\)](#page-9-3)

$$
F(\lambda_i, \chi_i) = (V_i(\rho)\chi_i(\rho), (C_i(\rho, \rho') - \lambda_i D_i(\rho, \rho'))\chi_i(\rho')) = 0
$$
\n(39)

where  $V_i(\rho)\chi_i(\rho) = (V_{0i}(\rho)\chi_i(\rho), V_{1i}(\rho)\chi_i(\rho), ...)$ <sup>T</sup>.

Then we use the iteration schemes [\(34\)](#page-8-0). The uniform grid with the nodes  $\Omega_h = {\zeta_0}$  $10^{-5}$ ,  $\zeta_{i+1} = \zeta_i + h$ ,  $\zeta_M = 0.999$ ,  $h = (\zeta_M - \zeta_0)/M$ } is used to approximate the finite interval  $0 \le \zeta = \rho/(1 + \rho) \le 1$  at  $M = 1500$  and  $h \approx 0.001$ . The eigenfunctions  $\chi_{ji}$  and the reaction matrix  $R_{ij}$  were calculated numerically for elastic scattering above the three-body threshold 3  $\rightarrow$  3. In the case of attraction  $c = -1$  we took the values of  $k = \sqrt{q^2 - \pi^2/36}$ corresponding to  $q = 0.6, 1.5$ . The repulsion case  $c = 1$  was considered at  $k = 0.1, 1.0$ . The approximation of problems [\(37\)](#page-9-3) and [\(39\)](#page-9-4) with six equations  $N = 6$  was used. The non-diagonal elements were calculated by means of equation [\(36\)](#page-9-1). Examples of calculated *R* matrices are demonstrated by [\(40\)](#page-9-5) and [\(41\)](#page-10-0) in the cases of  $c = -1$  at  $q = 0.6$  and  $c = 1$  at  $k = 0.1$ , respectively. Below, the factor *x* in brackets means  $(x) \equiv 10^x$ 

<span id="page-9-5"></span>
$$
\{R(c=-1, q=0.6)\}_{j,i=1}^{N=6}
$$

$$
= \begin{pmatrix} 1.29 & 2.97(-8) & 3.88(-7) & 6.59(-9) & -1.08(-7) & -1.61(-7) \\ 6.89(-8) & -0.59 & -3.28(-2) & -6.40(-3) & -2.27(-3) & -1.03(-3) \\ 3.70(-8) & -3.29(-2) & -0.63 & -4.14(-2) & -9.67(-3) & -3.81(-3) \\ 7.13(-8) & -6.43(-3) & -4.16(-2) & -0.63 & -4.28(-2) & -1.04(-2) \\ 1.10(-7) & -2.29(-3) & -9.78(-3) & -4.32(-2) & -0.63 & -4.27(-2) \\ 1.51(-7) & -1.06(-3) & -3.90(-3) & -1.06(-2) & -4.35(-2) & -0.62 \end{pmatrix}
$$
 (40)

<span id="page-10-1"></span>**Table 3.** The convergence of the values arctan  $R_{ii}$  of the  $R$  matrix, calculated by the iteration scheme [\(34\)](#page-8-0), versus the number *N* of equations [\(35\)](#page-9-2), are shown in the columns  $2-7$ , at the values of momentum *k* given in the first column. The eigenphase shifts  $\delta_{\text{eig}}^{R_{66}}$  [\(36\)](#page-9-1) of the matrix *R*, which are calculated by means of the iteration scheme [\(34\)](#page-8-0) for six equations [\(35\)](#page-9-2), are shown in the ninth column. For comparison, the values arctan  $R_{ij}^{\text{exact}}$  and the eigenphase shifts  $\delta_{\text{exact}}^{R_{\text{66}}}$  of the  $R_{\text{exact}}^{\text{exact}}$  matrix defined by equation [\(17\)](#page-4-1) via the matrix  $S_{\text{exact}}^{\text{exact}}$ , calculated using equation [\(19\)](#page-4-2) in approximation, are shown in columns 8 and 10, respectively. The asterisk is used to mark that the value  $\pi/4$  has been added to arctan  $R_{00}$ , as follows from the compatibility relation of the asymptotic boundary conditions [\(16\)](#page-4-0) and the asymptotic behaviour of [\(35\)](#page-9-2).

	N								
$\boldsymbol{k}$	$\mathbf{1}$	2	3	$\overline{4}$	5	6	arctan $R_{ii}^{\text{exact}}$	$\delta^{R_{66}}_{\rm eig}$	$\delta_\text{exact}^{R_{66}}$
	$c=-1$								
0.293	$2.920*$	$2.992*$	$3.006*$	$3.011*$	$3.014*$	$3.016*$	$3.023*$	$3.016*$	$3.023*$
		3.673	3.676	3.676	3.676	3.676	3.677	3.759	3.765
			3.698	3.703	3.703	3.703	3.706	3.717	3.723
				3.699	3.703	3.704	3.708	3.685	3.690
					3.698	3.702	3.709	3.663	3.669
						3.697	3.709	3.654	3.657
1.406	$2.047*$	$2.230*$	$2.268*$	$2.282*$	$2.289*$	$2.294*$	$2.313*$	$2.294*$	$2.313*$
		1.711	1.686	1.684	1.684	1.684	1.684	2.145	2.162
			1.760	1.732	1.731	1.730	1.731	1.931	1.948
				1.769	1.741	1.740	1.741	1.780	1.791
					1.769	1.742	1.742	1.685	1.691
						1.769	1.742	1.642	1.643
	$c=1$								
0.10	$-4.340$	$-4.340$	$-4.340$	$-4.340$	$-4.340$	$-4.339$	$-4.339$	$-4.331$	$-4.333$
		$-4.349$	$-4.348$	$-4.348$	$-4.348$	$-4.348$	$-4.349$	$-4.333$	$-4.336$
			$-4.348$	$-4.348$	$-4.348$	$-4.348$	$-4.350$	$-4.338$	$-4.341$
				$-4.348$	$-4.347$	$-4.347$	$-4.350$	$-4.346$	$-4.348$
					$-4.347$	$-4.347$	$-4.351$	$-4.356$	$-4.359$
						$-4.346$	$-4.351$	$-4.368$	$-4.371$
1.00	$-2.194$	$-2.167$	$-2.165$	$-2.165$	$-2.165$	$-2.165$	$-2.165$	$-2.101$	$-2.102$
		$-2.294$	$-2.257$	$-2.254$	$-2.254$	$-2.254$	$-2.255$	$-2.131$	$-2.131$
			$-2.298$	$-2.260$	$-2.257$	$-2.257$	$-2.259$	$-2.192$	$-2.189$
				$-2.299$	$-2.260$	$-2.257$	$-2.260$	$-2.280$	$-2.275$
					$-2.298$	$-2.259$	$-2.260$	$-2.394$	$-2.388$
						$-2.297$	$-2.260$	$-2.526$	$-2.524$

<span id="page-10-0"></span> ${R(c = 1, k = 0.1)}_{j,i=1}^{N=6}$ 



One can see that the matrices are symmetrical to three significant digits, which corresponds to the calculation accuracy of the order of  $10^{-3}$ . At  $c = -1$  the element  $R_{00}$  describes  $2 \rightarrow 2$ scattering. The non-diagonal elements  $R_{j0} = R_{0j}$ , corresponding to the transitions 2  $\rightarrow$  3 and  $3 \rightarrow 2$ , are zero to the above accuracy, i.e. there are no non-elastic scattering transitions in the case under consideration [\(21\)](#page-5-3). For  $3 \rightarrow 3$  scattering the non-diagonal elements  $R_{ji}$ 



<span id="page-11-0"></span>**Figure 1.** The bound state and half-bound state wavefunctions  $\Psi_b$  at  $2E_b \approx -\pi^2/9$  and  $\Psi_{hb}$  at  $2E_{hb} \approx -\pi^2/36$  ( $q \approx 0$ ) (upper figures). The scattering wavefunctions  $\Psi_0^s$  at  $q = \pi/6$  (i.e. at the three-body threshold energy  $2E = k^2 = 0$ ) for the attractive pair potentials  $c = -1$ , and  $\Psi_0^s$  at  $k = 0.6$  for the repulsive ones  $c = 1$  (lower figures).

are small at  $k < 1$  in accordance with the asymptotic expansion of the elements  $S_{ji}$  of the exact *S* matrix [\(19\)](#page-4-2). Correct consideration of the problem at  $k > 1$  requires a large number of equations, which is beyond the scope of the present paper, while at  $k \gg 1$  the diagonal approximation holds. In table [3](#page-10-1) the convergence of arctan  $R_{ii}$  calculated by means of the iteration scheme  $(34)$  with respect to the number *N* of equations  $(35)$  is shown in columns 2–7 at the values of the momentum *k* from the first column. The eigenphase shifts  $\delta^{R_{66}}_{\text{eig}}$  [\(36\)](#page-9-1) of the matrix *R* calculated by means of the iteration scheme [\(34\)](#page-8-0) for six equations ( $35$ ) are shown in the ninth column. For comparison the values arctan  $R_{ii}^{\text{exact}}$  and the eigenphase shifts *δ R*<sup>66</sup> exact of *R*exact matrix expressed by equation [\(17\)](#page-4-1) via the matrix *S*exact, calculated by means of equation [\(19\)](#page-4-2) in the six-state approximation, are shown in columns 8 and 10, respectively. In the case of  $c = -1$  the asterisk means that the value  $\pi/4$  was added to arctan  $R_{00}$ , as follows from the compatibility of the asymptotic boundary conditions [\(16\)](#page-4-0) and the asymptotic behaviour of [\(35\)](#page-9-2). With the number of equations growing up to  $N = 6$  the results converge to the analytical ones to the accuracy of three significant digits.

## **6. Conclusion**

We formulated the two-dimensional scattering problem in terms of the Schwinger variational functional, with the trial functions forming an adiabatic basis, as a spectral problem for a set of coupled one-dimensional integral equations. We elaborated stable iteration schemes to solve with prescribed accuracy the multi-channel spectral problem for a set of one-dimensional integral equations in the case of both discrete and continuous spectra. The efficiency of the proposed iteration schemes and their convergence with respect to the number of basis functions are studied in the exactly solvable model of three identical particles on a line with pair attraction and repulsion zero-range potentials both below and slightly above the three-body threshold. Figure [1](#page-11-0) (the first two plots) shows the wavefunctions  $\Psi_b(\rho, \theta)$  and  $\Psi_{hb}(\rho, \theta)$ 

for the bound state problem calculated by means of scheme [\(26\)](#page-6-0). Note that the necessity to account for states of the half-bound type arises, e.g., in calculations of loosely bound states of trimers of helium atoms [2, 3]. Figure [1](#page-11-0) (the second two plots) shows the wavefunctions  $\Psi_0^s(\rho, \theta)$  calculated using scheme [\(34\)](#page-8-0) above the three-body threshold for the scattering problems at  $q = \pi/6$  for  $c = -1$  and at  $k = 0.6$  for  $c = 1$ . The maxima and minima of these functions lie on pair collision lines, respectively. As one can see, the model under consideration preserves the most important characteristic features of the three-body problem as an interesting benchmark for the analysis of multichannel calculations. The approach developed allows a straightforward generalization over the multidimensional and multi-channel scattering problems by means of the appropriate choice of the representation of basis functions, boundary conditions, and approximate solutions of the set of coupled one-dimensional integral equations.

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## **References**

- [1] Demkov Yu N and Ostrovskii V N 1988 *Zero-Range Potentials and their Applications in Atomic Physics* (New York: Plenum)
- [2] Kolganova E A, Motovilov A K and Sofianos S A 1998 *J. Phys. B: At. Mol. Opt. Phys.* **31** 1279
- [3] Rudnev V and Yakovlev S 2000 *Chem. Phys. Lett.* **328** 97
- [4] Morse P M and Feshbach H 1953 *Methods of Theoretical Physics* vol 2 (New York: McGraw-Hill)
- [5] Chuluunbaatar O, Puzynin I V and Vinitsky S I 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** L425
- [6] Chuluunbaatar O, Puzynin I V and Vinitsky S I 2002 *J. Comput. Methods Sci. Eng.* **2** 37
- [7] Abrashkevich A A, Kaschiev M S and Vinitsky S I 2000 *J. Comput. Phys.* **163** 328
- [8] McGuire J B 1964 *J. Math. Phys.* **5** 622
- [9] McGuire J B and Hurst C A 1972 *J. Math. Phys.* **13** 1595
- [10] McGuire J B and Hurst C A 1988 *J. Math. Phys.* **29** 155
- [11] Albeverio S, Dabrowski L and Fei S M 2000 *Int. J. Mod. Phys.* B **14** 721
- [12] Albeverio S, Fei S M and Kurasov P 2002 *Preprint* quant-ph 0205145
- [13] Vinitsky S I, Larsen S Y, Pavlov D V and Proskurin D V 2001 *Phys. At. Nucl.* **64** 27
- [14] Gibson W, Larsen S Y and Popiel J J 1987 *Phys. Rev.* A **35** 4919
- [15] Kurasov P B and Melnikov Yu B 1989 *Topological Phases in Quantum Theory* ed B Markovski and S Vinitsky (Singapore: World Scientific) p 204
- [16] Popiel J J and Larsen S Y 1993 *Few-Body Systems* **15** 129
- [17] Amaya-Tapia A, Larsen S Y and Popiel J J 1997 *Few-Body Systems* **23** 87
- [18] Dubovik V M, Markovski B L, Suzko A A and Vinitsky S I 1989 *Phys. Lett.* A **142** 133
- [19] Sobolev S L 1963 *Applications of Functional Analysis in Mathematical Physics* (Providence, RI: American Mathematical Society)
- [20] Abramowitz M and Stegun I 1964 *Handbook of Mathematical Functions* (New York: US Govt Printing Office)