FEW-BODY QUANTUM PROBLEM IN THE
BOUNDARY-CONDITION MODEL

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Systems of three and four quantum particles in the boundary-condition model are considered. The Faddeev–Yakubovsky approach is applied to construct the Fredholm–type integral equations for these systems in framework of the Potential theory. The boundary–value problems are formulated for the Faddeev–Yakubovsky components of wave functions.

I. INTRODUCTION

The report is concerned with a treatment of three- and four-body quantum systems with pair interactions described by the boundary conditions of various types. Models of a such kind including the model of interactions with hard core attract attention due to simplicity of description of particle interaction at small distances (see Refs. [1], [2] for review). In these models, the repulsive part of the pair interaction is described by the boundary conditions for wave function which are set on a surface ∂ω in the (center of mass frame) two-body configuration space \( \mathbb{R}^n \). Here, \( n \) is dimension of particles (usually \( n = 3 \) and \( \partial \omega \) is a sphere in \( \mathbb{R}^3 \)).

However, being really simple in the two-body case, the boundary condition model in the case of three and more particles gives a birth to certain mathematical difficulties untypical for few-body problems with smooth potentials. Thing is that one comes here to necessity to construct a scattering theory in exterior of noncompact surface formed by aggregate of cylinders \( \partial \omega_\alpha \times \mathbb{R}^{(N-2)n} \) being supports in the \( N \)-body configuration space \( \mathbb{R}^{(N-1)n} \) for interactions in pair subsystems \( \alpha \). Standard equations of few-body scattering theory (see Ref. [3]) were derived for non-singular interactions and are not adjusted to a work with the arising boundary value problems. There are few attempts [4], [5] in physical literature to make an immediate regularization of these equations in three-body case using special limit procedures where at the beginning, one takes regular potentials with finite repulsive cores and then the cores are pulled to infinity. In their results, the papers [4], [5], [6] are close to this approach, too. These attempts were not quite successful because resulting equations were not of Fredholm type. To make the problem unique soluble it is necessary to take into account additional considerations [1], [8].

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Another method is proposed in works [9]–[11] of S.P.Merkuriev and author. Following the traditional approach to treatment of the boundary value problems for elliptic operators, we use the Potential theory (see Ref. [12]) reducing the problems to studies of integral equations on the surface where boundary conditions are set on. As mentioned above, this surface in the case of $N$-particle system with $N \geq 3$ is unbounded. Therefore, in a difference to the boundary value problems for compact surfaces, the equations of the Potential theory are not of Fredholm type. To transform them into those of Fredholm type we apply in three-body case, the method by L.D.Faddeev [13]. Namely we extract and inverse explicitly singular diagonal part of integral operator in the Potential equations. As a result we obtain the Faddeev-type equations for densities of simple and/or double layer (kind of densities depends on a type of boundary conditions) [9]–[11] which are did of Fredholm type and make possible to ground the scattering problem [11]. Note, in the recent works [14], a new method to prove the completeness of wave operators in $N$-body problems with arbitrary $N$ has been developed. This method is based on the concept of locally conjugate operator and is extended on the hard-core $N$-body Hamiltonians [15].

Alongside with the integral form we use also a differential form of the Potential equations. Here, a very important thing are the generalized potentials (quasipotentials) [2], [11] (one-dimensional variants of quasipotentials for the boundary-condition model were constructed for the first time in Refs. [16], [17]) allowing to reformulate boundary conditions in terms of singular distributions. These potentials are presented by linear combinations of the delta-function concentrated on the surface and its derivative with respect to the surface normal. The generalized potential method simplifies a scheme of derivation of the Faddeev-Yakubovsky-type integral (in framework of the Potential theory) as well as differential (in terms of quasipotentials) equations for components of resolvent and then for the wave operators. In the work [2] we formulate such equations in the cases of three and four particles. However the derivation may be spread also on the case of a system with arbitrary number of particles. As in [3], integral equations allow to study asymptotical boundary conditions for the Yakubovsky components of wave functions at large values of space variables. The formulations obtained of the boundary value problems for the Faddeev–Yakubovsky differential equations may be applied to study of concrete few-body systems in the boundary-condition model. Some results of computations of three-body scattering and bound-state energies are presented in Refs. [10], [18].

In the present work, we review the results from Refs. [9]–[11], [2] and [18] reformulating them for the case of arbitrary dimension of particles $n \geq 2$.

II. NOTATIONS

In the report, we restrict ourselves only to the cases of $N = 3$ and $N = 4$ particles. For the sake of simplicity we suppose all the particles to be spinless.

For description of three-body system we shall use the standard reduced relative coordinates $x_\alpha, y_\alpha, \alpha = 1, 2, 3$. For example in the case of $\alpha = 1$ these coordinates are expressed through the radius-vectors $r_i \in \mathbb{R}^n$ and masses $m_i$ of particles by the formulae

$$
x_1 = \left[ \frac{2m_2m_3}{m_2 + m_3} \right]^{1/2} (r_2 - r_3), \quad y_1 = \left[ \frac{2m_1(m_2 + m_3)}{m_1 + m_2 + m_3} \right]^{1/2} \left( r_1 - \frac{m_2r_2 + m_3r_3}{m_2 + m_3} \right),
$$
Relative coordinates are combined in $2n$-vectors $X = (x_\alpha, y_\alpha)$. A choice of coordinate pair fixes cartesian coordinate system in $\mathbb{R}^{2n}$.

In the case of four-body system, alongside with the index $\alpha$ denoting again a pair subsystem, we use also the index $a$ for partition of the system in two subsystems. If the pair $\alpha$ belongs to one of these subsystems, we write $\alpha \subset a$. As above, we introduce the relative coordinates $x_\alpha, y_\alpha, x_\alpha \in \mathbb{R}^n, y_\alpha \in \mathbb{R}^{2n}$. Here, $y_\alpha$ is a set of relative coordinates of the pair $\alpha$ considered as a whole and two particles in the rest. A detailed description of relative coordinates for four-body system can be found in Ref. [3].

In the boundary-condition model, the configuration space $\Omega$ of $N$-body system includes the points $X \in \mathbb{R}^{(N-1)n}$ satisfying conditions $x_\alpha \in \omega_\alpha$ for all indices $\alpha$ where $\omega_\alpha, \omega_\alpha \subset \mathbb{R}^n$, is the domain outside with respect to a piece-wise smooth closed compact surface $\partial \omega_\alpha \subset \mathbb{R}^n$. This $\partial \omega_\alpha$ is a surface where the boundary conditions are set on in the problem of two particles belonging to pair $\alpha$.

By $\Gamma_\alpha$ we denote the $[(N-1)n-1]$-dimensional cylinders in $\mathbb{R}^{(N-1)n}$ engendered by surfaces $\partial \omega_\alpha, \Gamma_\alpha = \partial \omega_\alpha \times \mathbb{R}^{(N-2)n} = \{X \in \mathbb{R}^{(N-1)n} : X = (x_\alpha, y_\alpha), x_\alpha \in \partial \omega_\alpha\}$.

Hamiltonian of $N$-body system is defined in $L^2_2(\Omega)$ by the expression

$$Hf(X) = \left(-\Delta_X + \sum_\alpha v_\alpha(x_\alpha)\right)f(X)$$

on the functions $f \in W^2_2(\Omega)$ satisfying the Dirichlet conditions (hard-core model)

$$f|_{\partial \Omega} = 0$$

or conditions of the third type

$$\left[\frac{\partial}{\partial n_X} + \tau_\alpha(x_\alpha)\right]f(X)\big|_{\partial \Omega \cap \Gamma_\alpha} = 0, \quad x_\alpha \in \partial \omega_\alpha, \quad \alpha = 1, 2, 3,$$

on the boundary $\partial \Omega$ of the domain $\Omega$. Smooth functions $\tau_\alpha(x_\alpha)$ are parameters of the model and are defined for $x_\alpha \in \partial \omega_\alpha$. Potentials $v_\alpha(x_\alpha)$ describe pair interactions of particles at $x_\alpha \in \omega_\alpha$ and are supposed to be smooth quickly decreasing functions.

### III. FADDEEV EQUATIONS FOR DENSITY OF SIMPLE LAYER

At the beginning, we consider the first approach [9, 10] to the boundary-condition model based immediately on the Potential theory [12]. We demonstrate it for the case of $N=3$ and conditions (1) supposing also that $v_\alpha \equiv 0, \alpha = 1, 2, 3$. In this case the kernel $R(X, X', z), X, X' \in \Omega$, of resolvent $R(z) = (H - z)^{-1}$ satisfies the identity (following from the Green formula):

$$R(X, X', z) = R_0(X, X', z) - \int_{\partial \Omega} d\sigma_S R_0(X, S, z) \frac{\partial}{\partial n_S} R(X, X' z),$$

(3)
with \( R_0(X, S, z) \), \( R_0(z) = (-\Delta_X - z)^{-1} \), the Green function of the Laplacian \(-\Delta_X\) in \( L_2(\mathbb{R}^{2n}) \) and \( n_S \) the normal to \( \partial\Omega \) directed in \( \Omega \). It follows from the representation \( \mathcal{F} \) that Green function \( R(z) \) is explicitly expressed in terms of its normal derivative \( \mu(Z, X', z) = \frac{\partial}{\partial n_S} R(S, X', z) \). The surface integral \( \int_{\partial\Omega} d\sigma_S R_0(X, S, z) \mu(S) \equiv U(X, z) \) in \( \mathcal{F} \) is the potential of simple layer \( \mathcal{S} \) with density \( \mu \). This potential is known to have finite normal derivatives \( \mathcal{S} \) in all the points \( S \) where surface \( \partial\Omega \) is smooth,

\[
\lim_{x \to S} \frac{\partial U}{\partial n_S} = \frac{1}{2} \mu(S) + \int_{\partial\Omega} \frac{\partial}{\partial n_S} R_0(S, S', z) \mu(S') d\sigma_S.
\]

Here, the up (low) sign \(-(+)\) corresponds to inside (outside) limit, i.e. \( X \in \Omega \) (\( X \in \mathbb{R}^{2n} \setminus \overline{\Omega} \)).

Differentiating Equation \( \mathcal{F} \) with respect to the normal \( n_S \) and taking into account relationship \( \mathcal{P} \), we obtain the following simple-layer potential equation for \( \mu(S) \):

\[
\frac{1}{2} \mu(S) + \int_{\partial\Omega} \frac{\partial}{\partial n_S} R_0(S, S', z) \mu(S') d\sigma_S = \frac{\partial}{\partial n_S} R_0(S, X', z).
\]

In this equation, the variables \( X' \) and \( z \) are fixed parameters. For compact integration surfaces, the potential integral equations are known to be of Fredholm type \( \mathcal{S} \). Equation \( \mathcal{F} \) however, is not of the Fredholm type because the surface \( \partial\Omega \) is unbounded.

Let us construct the Faddeev-type \( \mathcal{F} \) equations for the density \( \mu \).

First, we shall introduce some new notations. Let \( \Gamma_0 \) be the part of cylinder \( \Gamma_\alpha \) belonging to \( \partial\Omega \), \( \Gamma^e_\alpha = \Gamma_\alpha \cap \partial\Omega \). It is clear that \( \partial\Omega = \bigcup_\alpha \Gamma^e_\alpha \). We shall denote by \( \Gamma^i_\alpha \) the part of \( \Gamma_\alpha \) lying inside of \( \partial\Omega \), \( \Gamma^i_\alpha = \Gamma_\alpha \setminus \Gamma^e_\alpha \). Restriction \( \mu_\alpha = \mu|_{\Gamma^i_\alpha} \) will be called the Faddeev component of the density \( \mu \). It is convenient to consider these components as functions defined on the total cylinders \( \Gamma_\alpha \). Then, by \( \mu^i_\alpha \left( \mu^e_\alpha \right) \) we shall denote the part of \( \mu_\alpha(S) \) defined on \( \Gamma^i_\alpha \left( \Gamma^e_\alpha \right) \).

A concrete definition of internal parts \( \mu^i_\alpha \left( \mu^e_\alpha \right) \) of the densities \( \mu_\alpha \) will be given in the following paragraph.

In this notation, Equation \( \mathcal{F} \) may be rewritten as the system of three coupled equations,

\[
\frac{1}{2} P^e_\alpha \mu_\alpha = P^e_\alpha V_\alpha R_0 - P^e_\alpha V_\alpha R_0 \sum_{\beta=1}^{3} \mu^e_\beta
\]

with \( P^e_\alpha \left( P^i_\alpha \right) \) the operator of multiplication on the characteristic function of the set \( \Gamma^e_\alpha \left( \Gamma^i_\alpha \right) \) and \( V_\alpha R_0(z) \) the integral operator with kernel \( V_\alpha R_0(S, X', z) = \frac{\partial}{\partial n_S} R_0(S, X', z), S \in \Gamma_\alpha, X' \in \mathbb{R}^{2n} \). On the other hand, we use the equations \( \mathcal{F} \) to define the internal parts \( \mu^i_\alpha \) of the densities \( \mu_\alpha \) replacing \( P^e_\alpha \) with \( P^i_\alpha \). Total components \( \mu_\alpha \) satisfy the equations

\[
\frac{1}{2} \mu_\alpha = V_\alpha R_0 - V_\alpha R_0 \sum_{\beta=1}^{3} \mu^e_\beta.
\]

\( ^1 \)Remember that for \( -\Delta_X \) in \( L_2(\mathbb{R}^\nu) \), the Green function \( R_0(z) \) is given explicitly, \( R_0(X, X', z) = \frac{i}{4} \left( \frac{\sqrt{z}}{2\pi} \right) \frac{H^{(1)}_{(\nu-2)/2}(\sqrt{z}|X - X'|)}{|X - X'|^{(\nu-2)/2}} \), with \( H^{(1)} \) the Hankel function of the first type.
Further, following by the Faddeev method, we transfer diagonal terms with $\beta = \alpha$ to the left sides and inverse operators $\frac{1}{2}I + V_\alpha R_0$ appearing there. As a result we obtain the following equations \[11\], \[9\] for densities $\mu_\alpha$:

$$\mu_\alpha = V_\alpha R_\alpha + \frac{1}{2}V_\alpha \mu_\alpha - V_\alpha R_\alpha \sum_{\beta \neq \alpha} \mu_\beta. \quad (7)$$

Here, $R_\alpha(z)$ stands for the Green function of three-body system with only hard-core interaction in pair $\alpha$. Operator $V_\alpha \rho_\alpha$ has the kernel $V_\alpha \rho_\alpha(S, S', z) = \int_{\Gamma_\alpha} \frac{\partial}{\partial n} R_\alpha(S, S'', z) R_{\alpha N}^i(S'', S', z) d\sigma_S$ with $R_{\alpha N}^i$ the Green function for the Neumann problem inside of $\Gamma_\alpha$. Both kernels $V_\alpha R_\alpha$ and $V_\alpha \rho_\alpha$ are explicitly expressed in terms of two-body subsystem $\alpha$.

The equations obtained have been studied by methods of the Potential theory \[11\]. It was shown in particular that after some iterations, the integral operator corresponding to the right-hand part of (7) may be present as a sum of compact operator and another operator with norm smaller than one. The latter is engendered by a neighborhood of the ribs of the surface $\partial \Omega$ formed by intersection of cylinders $\Gamma_\alpha$. Therefore, the Fredholm alternative may be applied to these equations and properties of the density $\mu$ may be investigated. These properties being known, we study all the necessary properties of the Green function $R(z)$ \[11\]. The further procedure \[11\] of constructing the wave operators and studying their properties (completeness, orthogonality, asymptotics etc.) is quite analogous to that designed for three-body problems with smooth potentials \[3\].

Equations similar to (7), are obtained and studied also in the case of the conditions (2) and non-zero pair potentials $v_\alpha$ \[11\].

**IV. FORMALISM OF GENERALIZED POTENTIALS**

Another approach to construct the integral as well as differential equations for components of resolvent (and wave functions) uses the formalism of generalized potentials \[2\], \[11\]. Note that equation (4) may be considered as the Lippmann-Schwinger equation with (quasi)potential $V$ acting as $Vf = \delta_{\partial \Omega} \frac{\partial}{\partial n} f^e$. Here, $\delta_{\partial \Omega} \mu$ stands for generalized function (distribution) called simple layer \[13\] and $\frac{\partial}{\partial n} f^e$, for the limit values on $\partial \Omega$ (taking from $\Omega$ ) of the normal derivative $\frac{\partial}{\partial n} f$. Later, we shall use also notations $\frac{\partial}{\partial n} f^i$ for similar limit values taken from $\mathbb{R}^{(N-1)n} \setminus \Omega$, and $f^e, f^i$ for respective limit values on $\partial \Omega$ of the function $f$ itself. The generalized function $\delta_{\partial \Omega} \mu$ acts on in accordance with the rule $(\varphi, \delta_{\partial \Omega} \mu) = \int_{\partial \Omega} d\sigma_S \varphi(S) \mu(S)$. Analogous notations will be used also in the case when surface $\partial \Omega$ is replaced with cylinders $\Gamma_\alpha$.

Let us introduce the two-body generalized potentials $V_\alpha$, $V_\alpha f = \delta_{\Gamma_\alpha} \frac{\partial}{\partial n} f^e$, and consider instead of $H$ the new “operator” $\hat{H}$,

$$\hat{H} f(X) = -\Delta f(X) + \sum_\alpha V_\alpha f(X), \quad (8)$$

with $X$ running all the space $\mathbb{R}^{(N-1)n}$. Thereby we spread the domain of $H$ on functions defined outside as well as inside of the surface $\partial \Omega$. According to \[11\] one has to suppose
these functions and their derivatives to be continuous right up to surface $\Gamma_\alpha$, $\alpha = 1, 2, 3$. However, the breaks $f^e - f^i \neq 0$ and $\frac{\partial}{\partial n} f^e - \frac{\partial}{\partial n} f^i \neq 0$ must be allowed when $\Gamma_\alpha$ is crossed. Set of these functions in $W^2_2(\mathbb{R}^{(N-1)n} \setminus \bigcup_\alpha \Gamma_\alpha)$ will be denoted by $D$. Action of the Laplacian $-\Delta$ on $D$ has to be understood in a sense of distributions, 

$$-\Delta f = -\Delta_0 f + \sum_\alpha \delta_{\Gamma_\alpha} \left( \frac{\partial f^i}{\partial n} - \frac{\partial f^e}{\partial n} \right) + \sum_\alpha \frac{\partial}{\partial n} \left[ \delta_{\Gamma_\alpha} \left( f^i - f^e \right) \right], \tag{9}$$

where $\Delta_0$ stands for the usual Laplacian. With (9) one can easily see that substitution of $\mathcal{V}_\alpha$ into the Schrödinger equation leads to the two-sided boundary conditions on $\Gamma_\alpha$.

$$\frac{\partial}{\partial n} f^i \bigg|_{\Gamma_\alpha} = 0, \tag{10}$$

$$f^i \bigg|_{\Gamma_\alpha} = f^e \bigg|_{\Gamma_\alpha}. \tag{11}$$

This means [11] that if the spectral parameter $z$ is out of (discrete) spectrum of respective boundary value problems for domains engendered inside of $\mathbb{R}^{(N-1)n} \setminus \bigcup_\alpha \Gamma_\alpha$ due to intersection of cylinders $\Gamma_\alpha$ then the spectral problem $\hat{H} \Psi = z \Psi$ for $\hat{H}$ is equivalent to that for $H$. Therefore, the conditions (11) may be replaced outside of this spectrum with the generalized potentials $\mathcal{V}_\alpha$.

In the same way one can consider the model with third-type conditions (2). Generalized potentials in this case are following [11]: $\mathcal{V}_\alpha f = -\delta_{\Gamma_\alpha} (\tau_\alpha f^e) + \frac{\partial}{\partial n} (\delta_{\Gamma_\alpha} f^e)$ (see also [2]).

It is easily to include in this formalism usual potentials $v_\alpha$. The only necessary thing is the replacement of $\mathcal{V}_\alpha$ in (8) with $\mathcal{V}_\alpha + v_\alpha$.

**V. DIFFERENTIAL EQUATIONS FOR COMPONENTS**

In the formalism of generalized potentials, the components and differential equations for them are constructed in the same way as in the case of usual potentials [3].

For example, the Faddeev components of the bound-state $N$-body wave function $\Psi$ which are defined as $U_\alpha = -R_0(z)[v_\alpha + \mathcal{V}_\alpha] \Psi$, satisfy the Faddeev differential equations

$$(-\Delta_X + v_\alpha + \mathcal{V}_\alpha - z)U_\alpha = -(v_\alpha + \mathcal{V}_\alpha) \sum_{\beta \neq \alpha} U_\beta. \tag{12}$$

At $X \notin \bigcup_\beta \Gamma_\beta$, these equations turn into habitual form [3]

$$(-\Delta_X + v_\alpha - z)U_\alpha = -v_\alpha \sum_{\beta \neq \alpha} U_\beta. \tag{12}$$

Presence of generalized potentials generates two-sided boundary conditions for components $U_\alpha$ on cylinders $\Gamma_\alpha$. In the hard-core model [12] these conditions may be written as follows:

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2Excluding the points belonging to the intersections $\bigcup_{\alpha, \beta, \gamma \neq \alpha} (\Gamma_\beta \cap \Gamma_\gamma)$ of cylinders $\Gamma_\alpha$, $\alpha = 1, 2, 3$. 

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\[
\sum_{\beta} \frac{\partial U^i_{\beta}}{\partial n} \bigg|_{\Gamma_\alpha} = 0, \quad \sum_{\beta} U^e_{\alpha \beta} \bigg|_{\Gamma_\alpha} = 0, \quad (13)
\]

with \(\alpha\) running all the numbers of pairs (see Refs. [9], [10], [2] for details). Analogous conditions in the case of the model (2) read as

\[
\sum_{\beta} U^i_{\beta} \bigg|_{\Gamma_\alpha} = 0, \quad \left[ \left( \frac{\partial}{\partial n} + \tau_\alpha \right) \sum_{\beta} U^e_{\alpha \beta} \right] \bigg|_{\Gamma_\alpha} = 0, \quad (14)
\]

In the four-body problem, we introduce after Faddeev components, those of Yakubovsky,

\[
U_{\alpha a} = -G_\alpha (v_\alpha + V_\alpha) \sum_{\beta \neq a, \beta \subset a} U_{\beta a}, \quad (15)
\]

Boundary conditions for them may be written [2] in the form

\[
\frac{\partial \Psi_{\alpha a}^i}{\partial n} \bigg|_{\Gamma_\alpha} = 0, \quad \Psi_{\alpha a}^e \bigg|_{\Gamma_\alpha} = 0 \quad (16)
\]

in the hard-core model (1) and

\[
\Psi_{\alpha a}^i \bigg|_{\Gamma_\alpha} = 0, \quad \left( \frac{\partial \Psi_{\alpha a}^e}{\partial n} + \tau_\alpha \Psi_{\alpha a}^e \right) \bigg|_{\Gamma_\alpha} = 0 \quad (17)
\]

in the case of conditions (2). Here, \((\alpha, a)\) runs all the chains of partitions and \(\Psi_{\alpha a} = \sum_{\gamma \subset a} U_{\gamma a} + \sum_{\beta \neq a, \beta \subset a} \sum_{\beta \neq a} U_{\beta a} \).

Components of the scattering wave functions in the boundary-condition model satisfy the same equations (12) and (13) and boundary conditions (13,16) or (14,17). For the scattering processes, asymptotical boundary conditions as \(X \to \infty\) for the Faddeev components \((N=3)\) and for the Yakubovsky components \((N=4)\) are similar to those in the case of usual potentials [3], [18]. With these conditions, the boundary value problems (12,13) and (15,16) (or (12,14) and (15,17)) become uniquely soluble (at energies lying out of the discrete spectrum of the respective external problem for \(\partial \Omega\) and some internal problems for the domains formed by intersection of cylinders \(\Gamma_\alpha\)). Results of concrete three-body computations of \((2 \to 2, 3)\) scattering processes and bound-state energies may be found in Refs. [10], [18].

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