A new method of description of three-particle Coulombic systems

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Abstract. We present a method for treatment of three charged particles. The proposed method has universal character and is applicable both for bound and continuum states. A finite rank approximation is used for Coulomb potential in three-body system Hamiltonian, that results in a system of one-dimensional coupled integral equations. Preliminary numerical results for three-body atomic and molecular systems like H^-, He, $pp\mu$ and other are presented.

Keywords: three-body atomic systems, hyperspherical functions, finite rank operator, bound states
PACS: 03.65.Ge, 31.15.-p, 31.15.xj, 36.10.Ee

INTRODUCTION

The quantum three-body problem emerges in various fields of physics, and different methods of treating it are developed. However, there are no universal methods able to solve it in case of charged particles in the continuum. These problem is important in atomic and molecular physics and in nuclear astrophysics.

The main purpose of the work is to develop a procedure applicable to treatment of three charged particles in continuum. One of the ways to construct it is to make an approximation on operator level, i.e. in the Hamiltonian of three-body system under consideration. After that any boundary conditions can be used. The idea of our work was inspired by earlier paper of N. Aronszajn et al, who introduced the so-called method of intermediate Hamiltonians. This method was applied to calculate lower bounds for eigenvalues of some differential operators. N. W. Bazley and D. W. Fox applied it to He atom and other physical systems [1, 2]. They constructed sequence of intermediate Hamiltonians using finite rank operators. These operators are defined in the whole space of full Hamiltonian. In opposite to that we will apply finite rank approximation in a subspace of the three-body system Hamiltonian, namely in the angular space of hyperspherical variables. This results in a system of coupled one-dimensional integral equations.

In the following sections we review a method of intermediate Hamiltonians, hypersperical coordinates, derive system of integral equations and report the results of calculations.

HYPERSPHERICAL COORDINATES

There are different ways to formulate the three-body problem. We use hyperspherical coordinates, and in this section we give a brief review of them. Complete theory, derivations etc can be found, e.g., in [5].

We start with the three-body system Hamiltonian:

$$H = -\sum_{i=1}^{3} \frac{1}{2m_i}\nabla_i^2 + \sum_{i<j} V_{ij}(\mathbf{r}_i - \mathbf{r}_j), \tag{1}$$

where i enumerates different particles and corresponding sets od Jackobi coordinates.is a numb$\mathbf{r}_i$ is a position vector of the i-th particle. The scaled Jackobi coordinates are introduced as follows:

$$\begin{aligned} \mathbf{x}_i &= \left[\frac{m_j m_k}{m_j + m_k}\right]^{1/2} (\mathbf{r}_j - \mathbf{r}_k) \\ \mathbf{y}_i &= \left[\frac{m_i(m_j+m_k)}{m_1+m_2+m_3}\right]^{1/2} \left(-\mathbf{r}_i + \frac{m_j\mathbf{r}_j + m_k\mathbf{r}_k}{m_j+m_k}\right) \end{aligned} \tag{2}$$

and the Hamiltonian (1) takes the form

$$H = -\frac{1}{2}\nabla_{\mathbf{x}}^2 - \frac{1}{2}\nabla_{\mathbf{y}}^2 + V, \tag{3}$$

where $V = V_{13} + V_{23} + V_{31}$ — a sum of pair potentials. Taking $\mathbf{x}$ and $\mathbf{y}$ in spherical coordinates $(\mathbf{x},\mathbf{y}) \to (x,\theta_1,\varphi_1,y,\theta_2,\varphi_2)$, one obtains:

$$\hat{H} = -\frac{1}{2x^2}\frac{\partial}{\partial x}\left(x^2\frac{\partial}{\partial x}\right) - \frac{1}{2x^2}\Delta_{\Omega_1} - \frac{1}{2x^2}\frac{\partial}{\partial x}\left(x^2\frac{\partial}{\partial x}\right) - \frac{1}{2y^2}\Delta_{\Omega_2} + V, \tag{4}$$

Now let us introduce hyperspherical variables:

$$x = \rho\cos\alpha, \quad y = \rho\sin\alpha \tag{5}$$

Here ρ is hyperradius, α — hyperangle. Hamiltonian expressed in terms of this variables has the form:

$$\hat{H} = -\frac{1}{2}\left(\frac{\partial^2}{\partial\rho^2} + \frac{5}{\rho}\frac{\partial}{\partial\rho}\right) - \frac{1}{2\rho^2}\left[\frac{\partial^2}{\partial\alpha^2} + 4\cot 2\alpha\frac{\partial}{\partial\alpha} + \frac{1}{\cos^2\alpha}\Delta_{\Omega_1} + \frac{1}{\sin^2\alpha}\Delta_{\Omega_2}\right] + V \tag{6}$$

Angular part of a kinetic energy operator is the hypermomentum operator:

$$\hat{K} = \frac{\partial^2}{\partial\alpha^2} + 4\cot 2\alpha\frac{\partial}{\partial\alpha} + \frac{1}{\cos^2\alpha}\Delta_{\Omega_1} + \frac{1}{\sin^2\alpha}\Delta_{\Omega_2}, \tag{7}$$

and its eigenfunctions are hyperspherical harmonics:

$$\mathscr{Y}_K^{l_1 m_1 l_2 m_2}(\alpha,\Omega_1,\Omega_2) = c_K^{l_1 l_2}(\sin\alpha)^{l_1}(\cos\alpha)^{l_2} P_n^{(l_1+\frac{1}{2},l_2+\frac{1}{2})}(\cos 2\alpha) Y_{l_1 m_1}(\Omega_1) Y_{l_2 m_2}(\Omega_2), \tag{8}$$

where

$$c_K^{l_1 l_2} = \left[\frac{2n!(K+2)(n+l_1+l_2+1)!}{\Gamma(n+l_1+3/2)\Gamma(n+l_2+3/2)} \right]^{1/2}. \quad (9)$$

Let us consider system of three particles with masses m_1, m_2, m_3 and charges q_1, q_2, q_3. The Coulomb potential has the form:

$$V(\mathbf{x}, \mathbf{y}) = \frac{b_1}{x_1} + \frac{b_2}{x_2} + \frac{b_3}{x_3}, \quad (10)$$

where $b_i = \sqrt{\frac{m_j m_k}{m_j + m_k}} q_j q_k$. In hyperspherical coordinates:

$$V(\rho, \Omega) = \frac{1}{\rho} \left(\frac{b_1}{\cos\alpha_1} + \frac{b_2}{\cos\alpha_2} + \frac{b_3}{\cos\alpha_3} \right) \quad (11)$$

Here α_i — hyperangles corresponding to different sets of Jacobi coordinates.

FINITE RANK OPERATORS

Finite rank operators are widely used in different problems of mathematical physics. They allow one to reduce complexity of a problem and proceed to its solution. E.g., in [4] finite-rank operator was used to describe nuclear part of full Hamiltonian in a problem of low energy $\pi - {}^3He$ scattering.

N. W. Bazley and D. W. Fox used finite rank operators to calculate lower bounds of eigenvalues of Schrödinger eqution [1, 2]. Let us shortly review the method of intermediate Hamiltonians they used.

We suppose that full Hamiltonian H can be presented as a sum of H^0, that has known eigenvalues and eigenfunctions, and a positively definite H'. The exactly solvable Hamiltonian H^0 is assumed to have ordered discrete energy levels $E_1^0 \leq E_1^0 \leq ...$ below its continuum spectrum. The corresponding eigenfunctions are ψ_1^0, and we have

$$H^0 \psi_i^0 = E_i^0 \psi_i^0. \quad (12)$$

Since $H = H^0 + H'$, where H' is positively definite, $H^0 \leq H$ and $E_1^0 \leq E_1$. Thus, the full Hamiltonian H and H^0 are linked by a sequence of intermediate Hamiltonians:

$$H^0 \leq H^k \leq H^{k+1} \leq H. \quad (13)$$

To construct the Hamiltonians H^k, we introduce a system of k linearly independent functions $p_1, p_2, ..., p_k$. The set of functions $p_1, p_2, ...$ is defined in the whole space of definition of the Hamiltonian H. Projection of some wavefunction φ on these functions is given by

$$P^k \varphi = \sum_{i=1}^{k} \alpha_k p_k \quad (14)$$

The projection P^k increases with k:

$$0 \leq \langle \varphi | P^k \varphi \rangle \leq \langle \varphi | P^{k+1} \varphi \rangle \leq \langle \varphi | \varphi \rangle \tag{15}$$

$$0 \leq \langle \varphi | H' P^k \varphi \rangle \leq \langle \varphi | H' P^{k+1} \varphi \rangle \leq \langle \varphi | H' \varphi \rangle \tag{16}$$

From Eq. (16) we can see that $H'P^k \leq H'P^{k+1} \leq H'$, and we now define intermediate Hamiltonian as

$$H^k = H^0 + H'P^k \tag{17}$$

It is important to to emphasize that the finite rank operator H^k acts on the functions $p_1, p_2, ...$ in the same way as full Hamiltonian H:

$$H^k|i\rangle = H|i\rangle, \quad i = 1, \ldots, k \tag{18}$$

This is the main property of a some finite rank operators which we use in our work.

Following this idea, we construct such an operator in the angular space of definition of operator (7). The Coulomb potential in hyperspherical variables has the form $V(\rho, \Omega) = \frac{1}{\rho} f(\Omega)$, where $f(\Omega)$ is the angular part of potential. We use a finite rank approximation in it. Namely, the function $f(\Omega)$ is replaced by a finite rank operator:

$$f(\Omega) \to \hat{f}^N = \sum_{i,j}^{N} f|\varphi_i\rangle d_{ij} \langle \varphi_j | f \tag{19}$$

Here φ_j are some auxiliary functions defined in angular space, $d_{ij} = \langle \varphi_i | f | \varphi_j \rangle^{-1}$ — inverse matrix element.

FORMALISM

Here we derive a system of coupled one-dimensional integral equations using the finite rank approximation. Wavefunction of an arbitrary system in bound state satisfies the Schrödinger equation:

$$(H_0 + V)|\Psi\rangle = E|\Psi\rangle \tag{20}$$

Here H_0 is kinetic energy, V — interaction potential. This equation can be written in integral form using free Green function:

$$|\Psi\rangle = (E - H_0)^{-1} V|\Psi\rangle = -G_E V|\Psi\rangle \tag{21}$$

Let us rewrite it in coordinate representation:

$$\Psi(\mathbf{R}) = -\int d\mathbf{R}' G_E(\mathbf{R}, \mathbf{R}') V(\mathbf{R}') \Psi(\mathbf{R}'), \tag{22}$$

where $\mathbf{R} = (\mathbf{x}, \mathbf{y}) = (\rho, \Omega)$, and use the Coulombic potential: $V(\mathbf{R}) = \frac{1}{\rho} f(\Omega)$. We obtain integral equation for the wavefunction Ψ in hyperspherical coordinates:

$$\Psi(\rho, \Omega) = -\int \rho'^5 d\rho' d\Omega' G_E(\rho, \rho'; \Omega, \Omega') \frac{1}{\rho'} f(\Omega') \Psi(\rho', \Omega') \tag{23}$$

Using finite rank operator (19) instead angular part of potential $f(\Omega)$, we obtain representation for the wavefunction Ψ:

$$\Psi(\rho,\Omega) = -\sum_{i,j}^{N} \int \rho'^4 d\rho' d\Omega' G_E(\rho,\rho';\Omega,\Omega') f(\Omega') \varphi_i(\Omega')\, d_{ij} C_j(\rho'), \qquad (24)$$

where $C_j(\rho') = \int d\Omega'' \varphi_j(\Omega'') \Psi(\rho,\Omega'')$.

In order to obtain a system of integral equations for coefficients $C_i(\rho)$, we use integral operator: $\int d\Omega\, \varphi_k(\Omega) f(\Omega) \ldots$

$$C_k(\rho) = -\sum_{i,j}^{N} \int d\rho'\, \rho'^4 \int d\Omega\, d\Omega'\, \varphi_k(\Omega) f(\Omega) G_E(\rho,\rho';\Omega,\Omega') f(\Omega') \varphi_i(\Omega')\, d_{ij} C_j(\rho') \qquad (25)$$

or

$$C_k(\rho) = -\sum_{i,j} \int d\rho'\, M_{ki}(\rho,\rho') d_{ij} C_j(\rho'), \qquad (26)$$

$$M_{ki}(\rho,\rho') = \rho'^4 \int d\Omega\, d\Omega'\, \varphi_k(\Omega) f(\Omega) G_E(\rho,\rho';\Omega,\Omega') f(\Omega') \varphi_i(\Omega') \qquad (27)$$

The Green function $G_E(\mathbf{R},\mathbf{R}')$ has quite a simple form in Jacobi coordinates; an analytical expression for it is derived in [6]. However, it has the simplest form in the momentum representation. To exploit this we insert full sets of hyperspherical functions $\sum |\mathscr{Y}^{l_1 l_2}_{KLM}\rangle\langle\mathscr{Y}^{l_1 l_2}_{KLM}|$ into the matrix element 27 and use a hyperspherical representation for a wavefunction of free particles:

$$G_E(\mathbf{x},\mathbf{y}) = \iint \frac{d\mathbf{p}d\mathbf{q}}{(2\pi)^6} \exp(i\mathbf{p}\mathbf{x} + i\mathbf{q}\mathbf{y}) \frac{2m/\hbar^2}{p^2+q^2+\kappa^2},$$

We obtain

$$\frac{1}{(2\pi)^3} e^{i\mathbf{q}\mathbf{x}+i\mathbf{p}\mathbf{y}} = \frac{1}{(\kappa\rho)^2} \sum_{KLMl_1l_2} i^K J_{K+2}(\kappa\rho)\, \mathscr{Y}^{l_1 l_2}_{KLM}(\Omega_\rho)\, \mathscr{Y}^{l_1 l_2}_{KLM}(\Omega_\kappa),$$

where $\kappa^2 = p^2 + q^2$. This allows us to derive the three-body free Green function in hyperspherical representation:

$$\begin{aligned} G^K_E(\rho,\rho') &= \iint \mathscr{Y}^{l_1 l_2}_{KLM}(\Omega)\, G_E(\mathbf{R},\mathbf{R}')\, \mathscr{Y}^{l_1 l_2}_{KLM}(\Omega_\kappa) d\Omega\, d\Omega' = \\ &= \int_0^\infty \frac{\kappa\, d\kappa}{(2\pi)^3} \left(\frac{\rho'}{\rho}\right)^2 J_{K+2}(\kappa\rho) J_{K+2}(\kappa\rho') \frac{1}{\kappa^2 + 2mE} = \\ &= \frac{1}{(2\pi)^3} \left(\frac{\rho'}{\rho}\right)^2 \begin{cases} I_{K+2}(\kappa_0\rho) K_{K+2}(\kappa_0\rho'), & 0 \le \rho \le \rho' \\ K_{K+2}(\kappa_0\rho) I_{K+2}(\kappa_0\rho'), & 0 \le \rho' \le \rho \end{cases} \end{aligned}$$

Here $J_n(x)$, $I_n(x)$ and $K_n(x)$ are Bessel function and modified Bessel functions of first and second kind, respectively. Now we can calculate the kernels of integral equations ((25)):

$$M_{ki}(\rho,\rho') = \sum_{KLMl_1l_2} G^K_E(\rho,\rho') \langle\varphi_k|f|\mathscr{Y}^{l_1 l_2}_{KLM}\rangle\langle\mathscr{Y}^{l_1 l_2}_{KLM}|f|\varphi_i\rangle \qquad (28)$$

We derived a system of coupled one-dimensional integral equations (26). Now one need to calculate the kernel and solve this system numerically. At this stage of treating the Coulomb three-body problem the finite rank approximation makes it sufficiently easier.

CALCULATION AND RESULTS

We constructed the finite rank operator (19) using hyperspherical functions. They have been chosen for convenience, but one can use some other complete set of orthonormalized functions defined in angular space.

It is important to mention that the representation (25) for solution of Schrödinger equation is not a well known hyperspherical expansion. One can see it from the definition of $C_i(\rho)$.

We performed calculations using finite rank operators constructed on 1, 3 and 6 auxiliary functions. In calculation the kernel (28) we should summate an infinite number of terms, but we stopped at values of the hypermomentum K equal to 6, 10 and 14. In order to solve integral equations, the variables ρ and ρ' were discretized with 100 mesh points.

We calculated binding energies of the ground state of such systems: $He, H^-, H_2^+, pp\mu$ and $dd\mu$. Results of these calculations are presented in Table 1 and 1. Table 1 shows a convergence of calculated binding energies with K_{max} for finite rank operator(19) constructed on 6 auxiliary functions, Table 2 shows a convergence of calculated binding energies with the rank of operator N, when the summation stops at $K_{max} = 14$.

TABLE 1. Calculated and exact binding energies, eV

	E_{ex}, eV	$K_{max} = 6$	$K_{max} = 10$	$K_{max} = 14$
H^-	14.34	18	16.2	15.6
He	79.0	95	87	85
H_2^+	16.25	10,1	13.5	15.1
$pp\mu$	2782	1690	2290	2332
$dd\mu$	2988	1845	2195	2654

TABLE 2. Calculated and exact binding energies, eV

	E_{ex}, eV	$N = 1$	$N = 3$	$N = 6$
H^-	14.34	18.2	17.1	15.6
He	79.0	95	89	85
H_2^+	16.25	11	13.7	15.1
$pp\mu$	2782	1850	2101	2332
$dd\mu$	2988	1990	2480	2654

The exact energies are taken from [7].

CONCLUSION

Binding energies of different three-body Coulombic systems were calculated within a finite rank approximation method. The finite rank approximation is made in an angular part of potential in three-body Hamiltonian. This method was tested on some of these systems earlier in [3]. The results obtained shows it can be useful for solving the Coulombic three-body problem.

Calculations were performed at various conditions, i.e. different dimension of the finite rank operator, limit of inner summation, number of mesh points. Results demonstrate reasonable agreement with known values of binding energies. Accuracy of calculation can be improved by takin into account more terms.

We suppose the proposed method will be also applicable to three charged particles in continuum.

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