

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

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1 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 A. Weinstein [1], 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

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He atom and other physical systems [2,3]. 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, derive system of integral equations and report the results of calculations.

2 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 [6].

We start with the three-body system Hamiltonian:

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

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

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

and the Hamiltonian (1) takes the form

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

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

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

Now let us introduce hyperspherical variables:

$$x = \rho \cos \alpha, \quad y = \rho \sin \alpha \quad (5)$$

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

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

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

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

and its eigenfunctions are hyperspherical harmonics:

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

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.

3 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 [5] finite-rank operator was used to describe nuclear part of full Hamiltonian in a problem of low energy $\pi - {}^3\text{He}$ scattering.

N. W. Bazley and D. W. Fox used finite rank operators to calculate lower bounds of eigenvalues of Schrödinger equation [2, 3]. 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 $E_1^0 \leq E_2^0 \leq \dots$ below its continuum spectrum. The corresponding eigenfunctions are ψ_i^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, \dots, p_k . The set of functions p_1, p_2, \dots 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 :

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

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

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

$$H^k = H^0 + H' P^k \quad (17)$$

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

$$H^k |i\rangle = H |i\rangle, \quad i = 1, \dots, k \quad (18)$$

This is the main property of some finite rank operators which we will use below.

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:

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

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

4 Formalism

Here we derive a system of coupled one-dimensional integral equations using the finite rank approximation. Let us start with the Schrödinger equation:

$$(H_0 + V)|\Psi\rangle = E|\Psi\rangle \quad (20)$$

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

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

Let us rewrite it in coordinate representation:

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

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:

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

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

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

where $C_j(\rho') = \int d\Omega'' \varphi_j(\Omega'') f(\Omega'') \Psi(\rho, \Omega'')$ — new unknown functions.

In order to obtain a system of integral equations for functions $C_i(\rho)$, we use integral operator: $\int d\Omega \varphi_k(\Omega) f(\Omega) \dots$. As a result we obtain:

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

or

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

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

The Green function $G_E(\mathbf{R}, \mathbf{R}')$ has the simplest form in the momentum representation. Using the plane wave expansion:

$$\frac{1}{(2\pi)^3} e^{i\mathbf{q}\mathbf{x} + i\mathbf{p}\mathbf{y}} = \frac{1}{(\kappa\rho)^2} \sum_{KLMl_1l_2} i^K J_{K+2}(\kappa\rho) \mathcal{Y}_{KLM}^{l_1l_2}(\Omega_\rho) \mathcal{Y}_{KLM}^{l_1l_2}(\Omega_\kappa),$$

in

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

we obtain partial harmonics of free Green function:

$$\begin{aligned} G_E^K(\rho, \rho') &= \iint \mathcal{Y}_{KLM}^{l_1l_2}(\Omega) G_E(\mathbf{R}, \mathbf{R}') \mathcal{Y}_{KLM}^{l_1l_2}(\Omega_\kappa) d\Omega d\Omega' = \\ &= \int_0^\infty \frac{\kappa d\kappa}{(2\pi)^3} \left(\frac{\rho'}{\rho}\right)^2 J_{K+2}(\kappa\rho) J_{K+2}(\kappa\rho') \frac{1}{\kappa^2 + 2mE} = \\ &= \frac{1}{(2\pi)^3} \left(\frac{\rho'}{\rho}\right)^2 \begin{cases} I_{K+2}(\kappa_0\rho) K_{K+2}(\kappa_0\rho'), & 0 \leq \rho \leq \rho' \\ K_{K+2}(\kappa_0\rho) I_{K+2}(\kappa_0\rho'), & 0 \leq \rho' \leq \rho \end{cases} \end{aligned}$$

Here $J_n(x)$, $I_n(x)$ and $K_n(x)$ are Bessel function and modified Bessel functions of first and second kind, respectively, $\kappa^2 = p^2 + q^2$. Now we can calculate the kernels of integral equations (25):

$$M_{ki}(\rho, \rho') = \sum_{KLMl_1l_2} G_E^K(\rho, \rho') \langle \varphi_k | f | \mathcal{Y}_{KLM}^{l_1l_2} \rangle \langle \mathcal{Y}_{KLM}^{l_1l_2} | f | \varphi_i \rangle \quad (28)$$

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.

5 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 set of linearly independent 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.

Table 1 Calculated and precise binding energies, eV

	E_{pr}, eV	FRA	$K_{max} = 6$	$K_{max} = 10$	$K_{max} = 14$
H^-	14.34	N=1	25.0	20.0	18.2
		N=3	20.0	18.5	17.1
		N=6	18.0	16.2	15.6
He	79.0	N=1	102	98	95
		N=3	99	91	89
		N=6	95	87	85
H_2^+	16.25	N=1	7.3	10.0	11.0
		N=3	8.5	12.0	13.7
		N=6	10.1	13.5	15.1
$pp\mu$	2782	N=1	1050	1700	1850
		N=3	1360	2044	2101
		N=6	1690	2290	2332
$dd\mu$	2988	N=1	1200	1820	1990
		N=3	1540	2072	2480
		N=6	1845	2195	2654

The precise energies are taken from [7].

6 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 [4]. The results obtained shows it can be useful for solving the Coulombic three-body problem.

One can expect that this method will also be applicable to three charged particles in continuum, since the approximation (19) is made at the operator level, but not in the wavefunction.

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