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NEW POSSIBILITIES OF HARMONIC OSCILLATOR BASIS APPLICATION FOR CALCULATION OF THE GROUND STATE ENERGY OF A COULOMB NON-IDENTICAL THREE-PARTICLE SYSTEM

A. Deveikis

Vytautas Magnus University, Vileikos 8, LT-44404, Kaunas, Lithuania
E-mail: algirdas.deveikis@vdu.lt

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A new harmonic oscillator (HO) expansion method for calculation of the non-relativistic ground state energy of the Coulomb non-identical three-particle systems is presented. The HO expansion basis with different size parameters in the Jacobi coordinates instead of only one unique oscillator length parameter in the traditional treatment is introduced. This method is applied to calculate the ground state energy of a number of Coulomb three-particle systems for up to 28 excitation HO quanta. The obtained results suggest that the HO basis with different size parameters in the Jacobi coordinates could lead to significant increasing of the rate of convergence for the ground state energy than in the traditional approach.

Keywords: harmonic oscillator basis, ground state energy, three-particle systems, quantum systems with Coulomb potential

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1. Introduction

The consistent first principal theoretical descriptions of the many-particle quantum systems are not yet able to perform calculations with a larger number of particles due to the space and speed limitations of current computational facilities. The well-known representatives of the methods that provide a universal way of describing the many-particle quantum systems are based on the Faddeev [1], Faddeev–Jakubovsky [2], functional-differential equations approach [3], and quantum Monte Carlo calculations [4] or on the expansions in an appropriate basis, like the harmonic oscillator (HO) functions [5–7]. The principle of translational invariance is particularly important for an adequate theoretical formalism. For example, the bag model with the centre-of-mass motion corrections that are taken into account can provide sufficiently good predictions for magnetic moments of baryons [8].

This paper is devoted to the development of the HO expansion method which is widely used in the nuclear [9] and hadronic physics [10] calculations. The main advantage of the HO expansion is to allow systematic computations of all matrix elements of interest [11]. Another distinct feature of the HO basis that greatly reduces the complexity of calculations is its exceptional property to ensure translational invariance in finite subspaces (i.e. complete $N\hbar\omega$ spaces) formed with transition to intrinsic coordinates [12]. On the other hand, one of the major drawbacks of the HO expansion method is its slow rate of convergence for Coulomb-type long range interaction potentials. Therefore, the further progress in application of the HO expansion method for calculation of the many-particle quantum systems and particularly taking into account the Coulomb-type interactions should be supported by development of new significantly more effective calculation techniques.

The purpose of the present paper is to consider the first-principles approach, based on an expansion of the wave function in the HO functions with different size parameters (oscillator lengths) in the Jacobi coordinates for handling the non-relativistic ground energy calculation problem of the Coulomb three-body systems of three distinguishable particles. By contrast, the traditional approach actually provides only one unique oscillator length for all Jacobi coordinates. Recently, the HO basis with two intrinsic scales has been applied for evaluation of the ground state energy of a number of Coulomb three-body systems with two identical particles for zero HO excitation energy and shows a significant advantage over the traditional HO basis expansion [13]. It seems that intrinsic coordinates accompanied with individual variational size parameters are more adapted to better grasp the physical contents of the quantum systems.

The three-particle systems subjected to the Coulomb interaction are very abundant in the nature and are of great interest in many branches of physics: molecular, atomic, nuclear and hadronic physics among others. For example, $\mu^- d^+ t^+$ is known to catalyse nuclear fusion at room temperature [14]. Another important example is about the recently obtained discrepancy between different determinations of the proton radius, which initiated consideration of the weakly bound three-particle systems such as $e^- \mu^- p^+$ and $\mu^- p^+ p^+$ [15]. The investigation of the three-particle Coulomb systems are of topical importance to the quantum chemistry community as well [16, 17].

It should be noted that there exists a lot of different techniques for non-relativistic calculations of the three-particle Coulomb systems. The analytical methods are acknowledged for their predictive character and yield simple wave functions (usually possessing some of the correct functional properties), but, on other hand, demonstrate a rather modest accuracy (see, e.g. [18] and references therein). The exponential expansion based variation methods may produce highly sophisticated wave functions, built with a large number of basis functions, and lead to very accurate energies the precision of which may exceed 35 significant digits, i.e. yield numerical solutions to the Schrödinger equation hereafter named "exact" [19]. However, in spite of very accurate results, the wave functions in these types of calculations are constructed mostly by intuition and have to be optimized each time for every particular system of particles. This circumstance severely restricts the perspectives of this approach in application to systems with a larger number of particles. Accurate solutions of the Schrödinger equation are therefore only available for the systems with up to six particles [20].

This paper focuses particularly on the Coulomb interactions. The motivations behind this choice from the numerical point of view are twofold. First, since the convergence of the HO expansion for Coulomb-type potentials is extremely slow, the consideration of Coulomb systems may provide a sensitive test of the efficiency of the proposed method. Another reason for choosing this type of potential is the presence of essentially "exact" solutions to the Schrödinger equation of the three-particle Coulomb systems. Thus, the accuracy of the method may be easily evaluated. To our knowledge, the expansion method on the HO functions with different size parameters in the Jacobi coordinates for calculation of the Coulomb non-identical three-particle systems has not been previously applied. The efficiency of the theoretical formulation has been illustrated by calculation of the ground state energy of a number of Coulomb three-particle systems with non-identical particles. The results obtained in the basis with different sizes are compared with the ones calculated in the traditional basis with the same oscillator length for each Jacobi coordinate and with those given in the literature.

The structure of this paper is as follows. The details of the formalism are presented in the next section. In Section 3 we present the results of the ground state energy calculations for a number of three-particle atomic and molecular systems. Finally, the concluding remarks are given in Section 4.

2. Method

The non-relativistic Hamiltonian for the confined Coulomb non-identical three-particle system, with masses m_1, m_2 and m_3, and charges equal to Z_1, Z_2 and Z_3, can be written in terms of single-particle and two-particle operators

$$\hat{H}(\hat{r}_1,\hat{r}_2,\hat{r}_3) = -\frac{\hbar^2}{2m_1}\Delta_{\vec{r}_1} - \frac{\hbar^2}{2m_2}\Delta_{\vec{r}_2} - \frac{\hbar^2}{2m_3}\Delta_{\vec{r}_3} + \alpha\hbar c\left(\frac{Z_1 Z_2}{|\vec{r}_1-\vec{r}_2|} + \frac{Z_1 Z_3}{|\vec{r}_1-\vec{r}_3|} + \frac{Z_2 Z_3}{|\vec{r}_2-\vec{r}_3|}\right), \quad (1)$$

where α is the fine structure constant, and $\vec{r}_i$ is the ith particle radius vector in the laboratory reference frame. For correct treatment of the internal dynamics of a three-particle system, the translational invariant Jacobi coordinates are introduced:

$$\begin{cases} \vec{\xi}_0 = \dfrac{m_1\vec{r}_1 + m_2\vec{r}_2 + m_3\vec{r}_3}{m_1 + m_2 + m_3}, \\ \vec{\xi}_1 = \vec{r}_1 - \dfrac{m_2\vec{r}_2 + m_3\vec{r}_3}{m_2 + m_3}, \\ \vec{\xi}_2 = \vec{r}_2 - \vec{r}_3. \end{cases} \tag{2}$$

The reduced masses for these Jacobi coordinates will be defined by

$$\begin{aligned} &\nu_0 = m_1 + m_2 + m_3, \\ &\nu_1 = \frac{m_1(m_2 + m_3)}{\nu_0}, \ \nu_2 = \frac{m_2 m_3}{m_2 + m_3}. \end{aligned} \tag{3}$$

In this method, we introduce individual size parameters, one for each Jacobi coordinate (except for the centre of mass coordinate) instead of only one unique size parameter in the traditional approach:

$$\vec{\xi}_i = b_i\vec{\rho}_i. \tag{4}$$

Here b_i are the dimensionless harmonic oscillator length parameters indicated with the index i = 1, 2 of the reduced masses (3). These size parameters are defined by the usual expression

$$b_i^2 = \frac{\hbar}{\nu_i\omega_i}, \tag{5}$$

where ω_i are the alternative well-used harmonic oscillator parameters with a dimension of angular frequency. Instead of these parameters it is convenient to introduce two new variational parameters γ_i allowing us to rewrite the intrinsic Hamiltonian in the dimensionless energy quantities:

$$\gamma_i = \sqrt{\frac{\nu_i c^2}{\hbar\omega_i}}. \tag{6}$$

Finally, the intrinsic three-body Hamiltonian can be represented in terms of the dimensionless Jacobi coordinates, and in $\hbar\omega_2$ energy units (these units provide the greatest simplification) as

$$\begin{aligned} \frac{\hat{H}_{\text{intr.}}(\vec{\rho}_1, \vec{\rho}_2)}{\nu_2 c^2} &= -\frac{1}{2}\nu_{12}\frac{1}{\gamma_1^2}\Delta_{\rho_1} - \frac{1}{2}\frac{1}{\gamma_2^2}\Delta_{\rho_2} \\ &+ \frac{Z_1 Z_2\alpha}{\left|\dfrac{1}{\nu_{12}}\gamma_1\vec{\rho}_1 - \dfrac{\nu_2}{m_2}\gamma_2\vec{\rho}_2\right|} + \frac{Z_1 Z_3\alpha}{\left|\dfrac{1}{\nu_{12}}\gamma_1\vec{\rho}_1 + \dfrac{\nu_2}{m_3}\gamma_2\vec{\rho}_2\right|} + \frac{Z_2 Z_2\alpha}{\gamma_2\rho_2}, \end{aligned} \tag{7}$$

where $\nu_{12} = \nu_1/\nu_2$. It should be noted that no simplifying assumptions or approximations are made in the derivation of this Hamiltonian.

In order to avoid unnecessary recoupling of angular momenta, we introduce the HO basis functions of a three-particle system with the inner order of the vector coupling specified by the ket vector

$$\left|(\eta_1\lambda_1, \eta_2\lambda_2)\lambda_{12}m_{\lambda_{12}}\right\rangle. \tag{8}$$

In this notation η_i is the number of harmonic oscillator quanta and λ_i is the orbital angular momentum of the HO function depending on the ith Jacobi coordinate $\vec{\rho}_i$, here i = 1, 2. The λ_{12} and $m_{\lambda_{12}}$ are the total orbital angular momentum and the magnetic quantum number of the vector coupled state, respectfully. It should be stressed that due to the Coulombic character of the interaction potential the formulae for calculation of ground state energies could not depend on the spins of particles. Therefore, spin functions are absent in the vector coupled basis functions of Coulomb three-particle systems. This circumstance significantly reduces the dimensions of Hamiltonian matrices and facilitates the computations.

The matrix element of the first kinetic energy term of the Hamiltonian (7) between the coupled three-particle HO functions (8) may be evaluated applying the usual Racah technique [21] (see details in [13]):

$$\begin{aligned} &\left\langle(\eta_1\lambda_1, \eta_2\lambda_2)\lambda_{12}m_{\lambda_{12}}\right| -\frac{1}{2}\Delta_{\rho_1}\left|(\eta_1'\lambda_1', \eta_2'\lambda_2')\lambda_{12}m_{\lambda_{12}}\right\rangle \\ &= \delta_{\lambda_1,\lambda_1'}\delta_{\eta_2\lambda_2,\eta_2'\lambda_2'}\frac{1}{2}\left[(2\eta_1 + \lambda_1 + \frac{3}{2})\delta_{\eta_1',\eta_1}\right. \\ &+ \sqrt{\eta_1\left(\eta_1 + \lambda_1 + \frac{1}{2}\right)}\delta_{\eta_1',\eta_1-1} \\ &\left. + \sqrt{(\eta_1+1)\left(\eta_1 + \lambda_1 + \frac{3}{2}\right)}\delta_{\eta_1',\eta_1+1}\right]. \end{aligned} \tag{9}$$

The matrix element of the second kinetic energy term of the Hamiltonian (7) may be derived in a similar way:

$$\left\langle (\eta_1\lambda_1,\eta_2\lambda_2)\lambda_{12}m_{\lambda_{12}}\left|-\frac{1}{2}\Delta_{\rho_2}\right|(\eta_1'\lambda_1',\eta_2'\lambda_2')\lambda_{12}m_{\lambda_{12}}\right\rangle$$
$$=\delta_{\lambda_2,\lambda_2'}\delta_{\eta_1\lambda_1,\eta_1'\lambda_1'}\frac{1}{2}\left[(2\eta_2+\lambda_2+\frac{3}{2})\delta_{\eta_2',\eta_2}\right.$$
$$+\sqrt{\eta_2\left(\eta_2+\lambda_2+\frac{1}{2}\right)}\delta_{\eta_2',\eta_2-1}$$
$$\left.+\sqrt{(\eta_2+1)\left(\eta_2+\lambda_2+\frac{3}{2}\right)}\delta_{\eta_2',\eta_2+1}\right]. \quad (10)$$

Eventually, the matrix elements of the single-body Coulomb term of the Hamiltonian (7) may be calculated along the same lines as for kinetic energy terms:

$$\left\langle (\eta_1\lambda_1,\eta_2\lambda_2)\lambda_{12}m_{\lambda_{12}}\left|\frac{1}{\rho_2}\right|(\eta_1'\lambda_1',\eta_2'\lambda_2')\lambda_{12}m_{\lambda_{12}}\right\rangle$$
$$=\delta_{\lambda_2,\lambda_2'}\delta_{\eta_1\lambda_1,\eta_1'\lambda_1'}\left\langle \eta_2\lambda_2\left|\frac{1}{\rho_2}\right|\eta_2'\lambda_2'\right\rangle. \quad (11)$$

Here the integral on normalized radial HO wave functions is denoted by

$$\left\langle \eta_2\lambda_2\left|\frac{1}{\rho_2}\right|\eta_2'\lambda_2'\right\rangle=\int_0^\infty R_{\eta_2\lambda_2}(\rho_2)\frac{1}{\rho_2}R_{\eta_2'\lambda_2'}(\rho_2)\rho_2^2\mathrm{d}\rho_2. \quad (12)$$

This integral may be computed most easily by direct numerical integration.

For calculation of the expectation values of the two-body Coulomb operators of the Hamiltonian (7) we choose to express them in a single-body form. This may be accomplished by the orthogonal transformation to new Jacobi coordinates:

$$\begin{pmatrix}\vec{\rho}_1\\ \vec{\rho}_2\end{pmatrix}=\begin{pmatrix}\sqrt{\frac{d}{1+d}} & \sqrt{\frac{1}{1+d}}\\ \sqrt{\frac{1}{1+d}} & -\sqrt{\frac{d}{1+d}}\end{pmatrix}\begin{pmatrix}\vec{y}_0\\ \vec{y}_1\end{pmatrix}. \quad (13)$$

The same transformation to the new Jacobi coordinates should also be performed for the coupled three-particle HO functions (8) in the matrix elements of the two-body Coulomb operators. In the case of orthogonal transformations such a type of transition between wave functions may be accomplished by means of Talmi–Moshinsky brackets [22]

$$\left\{\varphi_{\eta_1\lambda_1}(\vec{\rho}_1)\otimes\varphi_{\eta_2\lambda_2}(\vec{\rho}_2)\right\}_{\lambda_{12}\mu_{\lambda_{12}}}$$
$$=\sum_{\varepsilon_0\sigma_0,\varepsilon_1\sigma_1}\left\{\varphi_{\varepsilon_0\sigma_0}(\vec{y}_0)\otimes\varphi_{\varepsilon_1\sigma_1}(\vec{y}_1)\right\}_{\lambda_{12}\mu_{\lambda_{12}}}$$
$$\cdot\left\langle\varepsilon_0\sigma_0,\varepsilon_1\sigma_1:\lambda_{12}\,|\eta_1\lambda_1,\eta_2\lambda_2:\lambda_{12}\right\rangle_d, \quad (14)$$

where ε_i and σ_i are the oscillator quanta and angular momentum quantum numbers for the ith Jacobi coordinate $\vec{y}_i$, and i = 0,1. The first two-body Coulomb operator of Hamiltonian (7) will depend only on one variable in the basis of new wave functions if the parameter d of the Talmi–Moshinsky brackets assumes the form

$$d_1=\left(\frac{\nu_1}{m_2}\frac{\gamma_2}{\gamma_1}\right)^2. \quad (15)$$

Then, the denominator of the first two-body Coulomb operator may be reduced:

$$\frac{1}{\nu_{12}}\gamma_1\vec{\rho}_1-\frac{\nu_2}{m_2}\gamma_2\vec{\rho}_2=C_1\vec{y}_1. \quad (16)$$

Here, the factor C_1 is introduced:

$$C_1=\frac{1}{\sqrt{1+\left(\frac{\nu_1}{m_2}\frac{\gamma_2}{\gamma_1}\right)^2}}\left(\frac{1}{\nu_{12}}\gamma_1+\frac{\nu_1\nu_2}{m_2^2}\frac{\gamma_2^2}{\gamma_1}\right). \quad (17)$$

Now, the matrix element of the first two-body Coulomb operator may be simplified similarly as the single-body terms of the Hamiltonian (7) and finally takes the form

$$\left\langle (\eta_1\lambda_1,\eta_2\lambda_2)\lambda_{12}m_{\lambda_{12}}\left|1/\left|\frac{1}{\nu_{12}}\gamma_1\vec{\rho}_1\right.\right.\right.$$
$$\left.\left.\left.-\frac{\nu_2}{m_2}\gamma_2\vec{\rho}_2\right|\right|(\eta_1'\lambda_1',\eta_2'\lambda_2')\lambda_{12}m_{\lambda_{12}}\right\rangle$$
$$=\frac{1}{C_1}\sum_{\varepsilon_0=0}^{\min(\eta_1+\eta_2,\eta_1'+\eta_2')}\sum_{\sigma_0=\varepsilon_0(-2)}^{0}$$
$$\sum_{\sigma_1=\min(\varepsilon_1,\varepsilon_1')(-2)}^{0}\left\langle\varepsilon_0\sigma_0,\varepsilon_1\sigma_1:\lambda_{12}\left|\eta_1\lambda_1,\eta_2\lambda_2:\lambda_{12}\right\rangle_{d_1}\right.$$
$$\cdot\left\langle\varepsilon_0\sigma_0,\varepsilon_1'\sigma_1:\lambda_{12}\left|\eta_1'\lambda_1',\eta_2'\lambda_2':\lambda_{12}\right\rangle\delta_1\cdot\left\langle\varepsilon_1\sigma_1\left|\frac{1}{y_1}\right|\varepsilon_1'\sigma_1\right\rangle\right., \quad (18)$$

where the summation parameters are under restrictions: $\varepsilon_1 = \eta_1 + \eta_2 - \varepsilon_0$; $\varepsilon'_1 = \eta'_1 + \eta'_2 - \varepsilon_0$;

$|\sigma_0 - \sigma_1| \le \lambda_{12} \le \sigma_0 + \sigma_1$; $m_{\lambda_{12}}$ may take any allowed value for the given λ_{12}; $(-1)^{\eta_1+\eta_2} = (-1)^{\eta_1'+\eta_2'}$; the step of the summation indices σ_0 and σ_1 is minus two due to the relation $\varepsilon = 2n + \sigma$ between the number of harmonic oscillator quanta ε, the principal oscillator quantum number $n = 0, 1, 2...$ and the quantum number of the orbital angular momentum σ; $(-1)^{\lambda_1+\lambda_2} = (-1)^{\lambda_1'+\lambda_2'} = \pi = (-1)^{N_{\max}}$. The last relation contains the parity π of the coupled three-particle HO function (8), and the parameter $N_{\max}$ that measures the maximal allowed HO excitation energy (the model space truncation parameter). In the computation of the Hamiltonian matrix we always consider all the basis states with a number of quanta less or equal to the given number $N_{\max}$ ($\Sigma\eta_i \le N_{\max}$ and $\Sigma\varepsilon_i \le N_{\max}$). Actually, this is a usual prescription of the HO expansion methods. Similarly, the second two-body Coulomb operator of the Hamiltonian (7) will depend only on one variable in the new basis if the parameter d of the Talmi–Moshinsky brackets will be

$$d_0 = \left(\frac{m_3}{\nu_1}\frac{\gamma_1}{\gamma_2}\right)^2. \tag{19}$$

Then the denominator of the second two-body Coulomb operator takes the form

$$\frac{1}{\nu_{12}}\gamma_1\vec{\rho}_1 + \frac{\nu_2}{m_3}\gamma_2\vec{\rho}_2 = C_0\vec{y}_0, \tag{20}$$

where the factor C_0 is introduced:

$$C_0 = \frac{1}{\sqrt{1+\left(\frac{m_3}{\nu_1}\frac{\gamma_1}{\gamma_2}\right)^2}}\left(\frac{\nu_2}{m_3}\gamma_2 + \frac{m_3}{\nu_1\nu_{12}}\frac{\gamma_1^2}{\gamma_2}\right). \tag{21}$$

Finally, the matrix element of the second two-body Coulomb operator acquires the form

$$\left\langle (\eta_1\lambda_1,\eta_2\lambda_2)\lambda_{12}m_{\lambda_{12}}\left|1/\left|\frac{1}{\nu_{12}}\gamma_1\vec{\rho}_1 + \frac{\nu_2}{m_3}\gamma_2\vec{\rho}_2\right|\right|(\eta_1'\lambda_1',\eta_2'\lambda_2')\lambda_{12}m_{\lambda_{12}}\right\rangle$$

$$= \frac{1}{C_0}\sum_{\varepsilon_1=0}^{\min(\eta_1+\eta_2,\eta_1'+\eta_2')}\sum_{\sigma_1=\varepsilon_1(-2)}^{0}$$

$$\sum_{\sigma_0=\min(\varepsilon_0,\varepsilon_0')(-2)}^{0}\left\langle \varepsilon_0\sigma_0,\varepsilon_1\sigma_1:\lambda_{12}\middle|\eta_1\lambda_1,\eta_2\lambda_2:\lambda_{12}\right\rangle_{d_0}$$

$$\cdot\left\langle \varepsilon_0'\sigma_0,\varepsilon_1\sigma_1:\lambda_{12}\middle|\eta_1'\lambda_1',\eta_2'\lambda_2':\lambda_{12}\right\rangle_{d_0}\cdot\left\langle \varepsilon_0\sigma_0\left|\frac{1}{y_0}\right|\varepsilon_0'\sigma_0\right\rangle, \tag{22}$$

where $\varepsilon_0 = \eta_1 + \eta_2 - \varepsilon_1$ and $\varepsilon_0' = \eta_1' + \eta_2' - \varepsilon_1$. The restrictions of other summation parameters coincide to that of (18).

3. Results

In the presented method the ground state energy calculation process consists of a sequence of diagonalizations of the Hamiltonian (7) for different sets of the nonlinear parameters γ_1 and γ_2 while searching for the set that minimizes its lowest eigenvalue. The matrix of this Hamiltonian is calculated in the basis (8), truncated by a chosen maximal number of excitation HO quanta $N_{\max}$. Therefore, this minimum of the lowest eigenvalue with respect to nonlinear parameters obtained for each fixed $N_{\max}$ will be called the ground state energy and denoted thereafter as $E_{\max}$. The rate of convergence for the ground state energy will be evaluated as the rate at which the sequence of $E_{\max}$ values approaches the "exact" numerical ground state energy value with increasing of the dimension of the model space determined by the number $N_{\max}$.

Application of the method developed in this paper for calculation of the non-relativistic ground state energy $E_{\max}$ of the Coulomb three-particle systems with non-identical particles in the zeroth order approach, i.e. $N_{\max} = 0$, should be illustrated. In this case, the Hamiltonian matrix has only one matrix element and the variational procedure for the calculation of $E_{\min}$ is simplified to the minimization of a simple function with respect to two nonlinear parameters. Due to the simplicity of zeroth order computations they may be useful for a quick evaluation of nonlinear variational parameters and the ground state energy. The minimization procedure was implemented by our modified Golden section search method [23] alternatively for the parameters γ_1 and γ_2. This method was chosen for its well-known stability and was applied for the zero $N_{\max} = 0$ as well as for higher excitations $N_{\max} > 0$. In the zeroth order approach, the single matrix element under minimization takes the form

$$\left\langle 0\left|\frac{\hat{H}_{\text{intr.}}(\vec{\rho}_1,\vec{\rho}_2)}{\nu_2 c^2}\right|0\right\rangle = \frac{3}{4}\nu_{12}\frac{1}{\gamma_1^2}+\frac{3}{4}\frac{1}{\gamma_2^2} + \frac{2Z_1Z_2\alpha}{\sqrt{\pi}C_1}+\frac{2Z_1Z_3\alpha}{\sqrt{\pi}C_0}+\frac{2Z_2Z_3\alpha}{\sqrt{\pi}\gamma_2}. \quad (23)$$

It should be noted that in the zeroth order approach all quantum numbers of bra and ket states are equal to zero.

The ground state energy for a wide-range of the Coulomb three-particle systems with distinguishable particles has been calculated. The considered three-particle systems consist of the following elementary particles: electron e, muons $\mu^{\pm}$ and mesons $K^{\pm}$, proton p, deuteron d, tritium t. We have used the following internationally recommended masses of these particles as given by CODATA [24]: m_e = 0.510998918 MeV, m_μ = 105.65836668 MeV, m_K = 493.66 MeV, m_p = 938.272046 MeV, m_d = 1875.612859 MeV, and m_t = 2808.290906 MeV. The results of calculations for the zero order ground state energy $E_{\min}$ of the considered three-particle systems are presented in Table 1. It should be noted that in this method the variational procedure splits the partitions of particles into three groups concerning the permutation of their indices. For example, the label $m_1\{m_i\, m_j\}$ denotes that in this formulae m_1 should be equal to the mass of the lightest particle, $m_2\{m_i\, m_j\}$ means that m_1 should be substituted by the mass of the middleweight particle, and $m_3\{m_i\, m_j\}$ assigns m_1 to the mass of the heaviest particle. In the case of a system consisting of a K meson, a deuteron and a tritium, the label $m_1\{m_i\ m_j\}$ indicates that m_1 is equal to the mass of K meson, $m_2\{m_i\, m_j\}$ means that m_1 is equal to the mass of deuteron and $m_3\{m_i\ m_j\}$ designates that m_1 is equal to the mass of tritium. The permutation of the second and third particles in the list does not have any influence to the variational procedure results. The charges on each particle were set as $\{Z_1 = -1, Z_2 = +1, Z_3 = +1\}$, although reversing the charges (in the case of antiparticles) would produce the same eigenvalues due to the charge inversion invariance. According to this analysis, despite the highest values of the obtained ground state energies in the zeroth order approach, only the partition $m_1\{m_i\ m_j\}$ provides the highest rate of convergence to the "exact" values for higher excitations. The calculation of the ground state energy $E_{\min}$ with $N_{\max} = 0$ for the $m_2\{m_i\ m_j\}$ and $m_3\{m_i\ m_j\}$ partitions produces the same minimizing values of parameters $\gamma_1 = \infty$ and $\gamma_2 = 182$ for all considered three-particle systems. This asymptotic behaviour of the energy when one of the nonlinear parameters is large may be used for a quick indication of an inadequate partition (not with the highest rate of convergence) in this method. The accuracy of the obtained zeroth order results for the three-particle systems amounts only to 60–70% of the "exact" reference values [25–29].

Table 1. The ground state energies $E_{\min}$ (in eV) of the Coulomb three-particle systems with non-identical particles obtained for zero excitation HO energy ($N_{\max} = 0$). All ground state energies calculated for the $m_2\{m_i\, m_j\}$ and $m_3\{m_i\, m_j\}$ partitions of the particles have the same minimizing values of parameters: $\gamma_1 = \infty$ and $\gamma_2 = 182$. The "exact" numerical ground state energies of the three-particle systems are also indicated.

System	$m_1\{m_i\, m_j\}$			$m_2\{m_i\, m_j\}$ $E_{\min}$	$m_3\{m_i\, m_j\}$ $E_{\min}$	E_{exact}
	γ_1	γ_2	$E_{\min}$			
$e\mu K$ [25]	189	$6.66\cdot10^4$	–10.669	–11.537	–11.493	–16.035
epd [25, 26]	193	$4.04\cdot10^5$	–10.274	–11.546	–11.543	–16.270
ept [25, 26]	191	$4.85\cdot10^5$	–10.457	–11.547	–11.543	–16.271
edt [25, 26]	194	$7.05\cdot10^5$	–10.184	–11.547	–11.546	–16.303
μKp [25, 27]	211	$1.28\cdot10^3$	–1800.5	–2146.3	–1967.0	–2651.5
μKd [25, 27]	202	$1.65\cdot10^3$	–1971.0	–2260.6	–1967.0	–2761.6
μpd [25, 28]	203	$2.24\cdot10^3$	–1945.0	–2260.6	–2146.3	–2884.7
μpt [25, 28]	199	$2.63\cdot10^3$	–2020.4	–2301.4	–2146.3	–2925.1
μdt [25, 29]	200	$3.70\cdot10^3$	–1994.5	–2301.4	–2260.6	–3030.4
Kdt [25]	218	$1.00\cdot10^3$	–7867.8	–9489.1	–8832.4	–11695

This is significantly worse than in the case of two-particle systems, where the accuracy of the zeroth order HO expansion results in about 80% [30]. Since the least accurate mass value used is known to be 6 significant figures ($K^{\pm}$ meson), all energies are converged to the same number of significant figures as well. The number of significant digits of nonlinear parameters was judged from the energy convergence behaviour and, due to its flat character at minimum, may contain only 3 significant figures to provide the chosen precision of energy convergence.

The traditional approach based on the HO basis assumes that the harmonic oscillator wave functions have the same size (or the same scale) in all Jacobi coordinates. The proposed approach transforms to the traditional one with the simple substitution $\gamma_1 = \gamma_2 = \gamma$. According to the obtained results, the minimal value of the zeroth order ground state energy of all considered three-particle systems calculated within the framework of the traditional approach turns out to be infinitesimally small but positive. This illustrates a distinct advantage of the presented method over the traditional approach for calculation of the zero order ground state energy of the Coulomb three-particle systems with non-identical particles.

The performance of the developed method was examined by calculation of the ground state energy of the chosen three-particle systems for up to $N_{max} = 28$ excitation HO quanta. The rate of energy convergence for the $m_1\{m_i\, m_j\}$ partition is illustrated in Table 2 for the case of the *Kdt* system. The first two columns tabulate the number of excitation HO quanta N_{max} and the dimension of the corresponding Hamiltonian matrix H_{dim}. The two columns indicated by $H(\gamma)$ present the ground state energies E_{min} calculated within the framework of the traditional approach and the values of parameter γ chosen to minimize the corresponding ground state energy. Here the dashes in the row for the zero excitation HO energy indicate absence of meaningful physical results (the negative value of energy). The next three columns indicated by $H(\gamma_1, \gamma_2)$ display the ground state energies E_{min} and the values of nonlinear variational parameters, γ_1 and γ_2, which give the lowest values of the corresponding ground state energy.

The obtained results are in line with the well-known fact that the convergence of variational energy calculations of many-particle systems with Coulomb interaction in the HO basis is very slow. However, in general, the presented method demonstrates an overall significant improvement in the ground state energy calculation results compared with the traditional approach.

As noted previously, our ground state energy calculation results depend on the chosen partition of the particles. The permutation of the particle indices in the partition is equivalent to choosing different Jacobi coordinate sets for systems of three arbitrary particles [31]. So, the Jacobi coordinates introduced in this work (2) give a particular status to the first particle with respect to the other two particles. If the dimension of the basis would be infinite ($N_{max} = \infty$), the choice of the partition would

Table 2. The dependence of the ground state energy E_{min} (in eV) of the *Kdt* system for the partition $m_1\{m_i\, m_j\}$ on the number of excitation HO quanta N_{max}. The minimizing values of parameters γ, γ_1 and γ_2, and the dimension of the Hamiltonian (7) matrix H_{dim} are also indicated. The "exact" numerical ground state ener'gy for the *Kdt* system is –11695 eV [25].

N_{max}	H_{dim}	$H(\gamma)$		$H(\gamma_1, \gamma_2)$		
		γ	E_{min}	γ_1	γ_2	E_{min}
0	1	–	–	218	1000	–7867.9
4	10	517	–4514.7	179	705	–10131
8	35	391	–7814.1	161	660	–10863
12	84	352	–9204.5	151	637	–11183
16	165	330	–9917.6	142	607	–11353
20	286	313	–10380	134	585	–11453
24	455	305	–10690	131	557	–11516
28	680	299	–10897	128	542	–11558

be irrelevant. However, for the truncated expansion there exists a special partition ($m_1\{m_i\ m_j\}$ in our case), which gives better results. The variational surfaces of the ground state energy for each system also depend on the adopted partition. In Fig. 1 the variational surfaces of the ground state energy of *Kdt* system for the $m_2\{m_i\ m_j\}$ and $m_3\{m_i\ m_j\}$ partitions calculated with 16 excitation HO quanta ($N_{\max} = 16$) are shown. The obtained variational surfaces have the global minimum and the valley passing through the saddle point to another valley that is sloping downward as the value of γ_1 is increasing. Usually the global minimum is absent for these partitions if the number of excitation HO quanta is not large enough. The dependence of the variational surface of the ground state energy of *Kdt* system for the partition $m_1\{m_i\ m_j\}$ on the number of excitation HO quanta $N_{\max}$ is shown in Fig. 2. The variational surface for the partition $m_1\{m_i\ m_j\}$ in general is similar to that for the partitions $m_2\{m_i\ m_j\}$ and $m_3\{m_i\ m_j\}$, except that γ_1 and γ_2 are swapping roles (the valley is passing along the γ_2 direction), the global minimum is lower and the saddle point in this case is located significantly higher and further away. For these reasons we chose to present the variational surfaces for

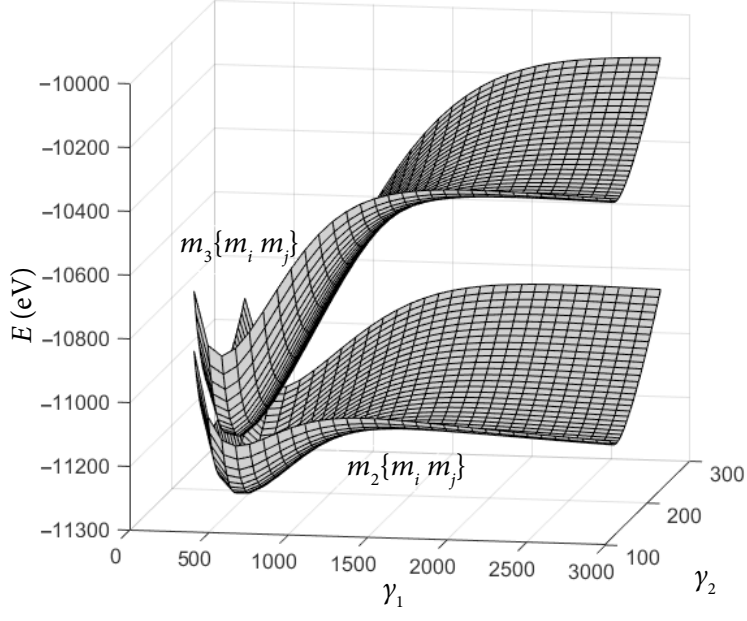

Fig. 1. Variational surfaces of the ground state energy of the *Kdt* system at $N_{\max} = 16$ plotted against the nonlinear parameters γ_1 and γ_2 for the $m_2\{m_i\ m_j\}$ and $m_3\{m_i\ m_j\}$ partitions.

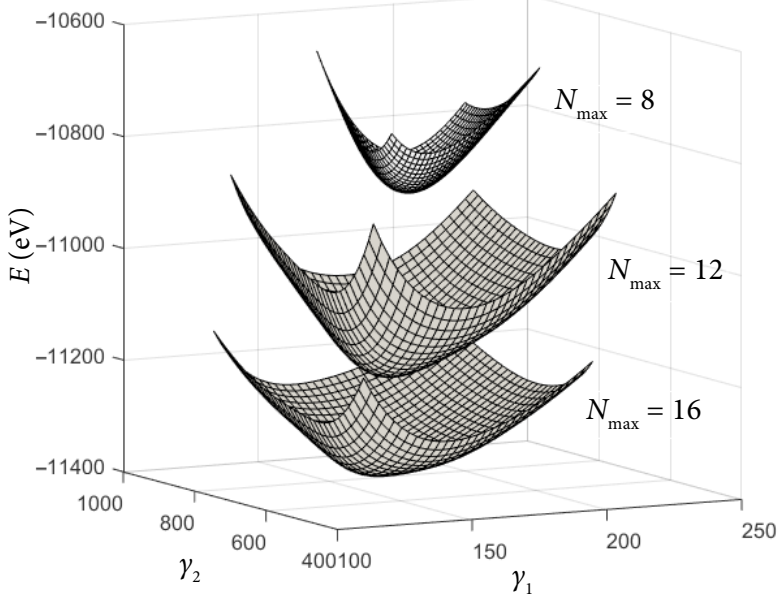

Fig. 2. Variational surfaces of the ground state energy of the *Kdt* system at $N_{\max} = 8, 12, 16$ plotted against the nonlinear parameters γ_1 and γ_2 for the partition $m_1\{m_i\ m_j\}$.

the partition $m_1\{m_i\ m_j\}$ and the ones for the other two partitions in two different figures. The investigation shows that the variational calculation of the ground state energy of three-particle systems for different partitions gives converging ground state energy values when the dimension of the basis increases.

Table 3 illustrates the accuracy of calculations by computing the ground state energy $E_{\min}$ for the chosen Coulomb three-particle systems of non-identical particles with 28 excitation HO energy ($N_{\max} = 28$) and for the $m_1\{m_i\ m_j\}$ partition. The first column of this table indicates the symbols of the three-particle systems considered, the next two columns indicated by $H(\gamma)$ contain the ground state energies $E_{\min}$ calculated within the framework of the traditional approach and the values of the parameter γ chosen to minimize the corresponding ground state energy. Here the dashes indicate absence of meaningful physical results (the negative value of energy). The next three columns indicated by $H(\gamma_1, \gamma_2)$ tabulate the ground state energies $E_{\min}$ and values of variable parameters, γ_1 and γ_2, which give the lowest values of the corresponding ground state energy. The following column shows the lowest energy threshold E_{th} of the Coulomb three-particle systems under consideration (see below Eq. (24)). The last column presents the "exact" numerical ground state energies [25–29]. The obtained ground state energy calculation results for the considered three-particle systems are on the average 1% higher than the "exact" reference values, however, significantly lower than in the traditional approach.

According to these calculation results, all the three-particle systems presented in Table 3 satisfy the stability condition [16, 32], i.e. their ground state energy is below the lowest energy threshold defined as the lowest ground state energy of the separate two-body subsystem

$$E_{\text{th}} = -\frac{1}{2}\frac{m_1 m_3}{m_1 + m_3}(c\alpha Z_1 Z_3)^2, \tag{24}$$

where m_1 denotes the lightest particle and m_3 is the heaviest particle of the three-particle system. Therefore, the proposed method correctly gives the bounding of the ground state for these systems. The obtained results indicate that this method may be applied to the studies of the stability of the three-particle systems except the weakly bound ones.

The analysis of the bound state problem of Coulomb three-particle systems with non-identical particles with the presented method shows its distinct advantages over the traditional approach. First, the ground state energies calculated with different sizes in the Jacobi coordinates are significantly lower than those calculated with only one size parameter for all Jacobi coordinates. Second, the proposed method correctly predicts negative values of the ground-state energies of all the Coulomb

Table 3. The ground state energies $E_{\min}$ (in eV) for the Coulomb three-particle systems with non-identical particles calculated for the $m_1\{m_i\ m_j\}$ partition and 28 excitation HO quanta ($N_{\max} = 28$). The minimizing values of parameters γ, γ_1 and γ_2, the lowest energy thresholds and the "exact" numerical energies of the ground states are also indicated.

System	$H(\gamma)$		$H(\gamma_1, \gamma_2)$			E_{th}	E_{exact}
	γ	$E_{\min}$	γ_1	γ_2	$E_{\min}$		
eμK [25]	–	–	108	$1.59\cdot10^4$	−15.929	−13.592	−16.035
epd [25, 26]	–	–	103	$1.09\cdot10^5$	−16.179	−13.602	−16.270
ept [25, 26]	–	–	104	$1.20\cdot10^5$	−16.180	−13.603	−16.271
edt [25, 26]	–	–	102	$2.11\cdot10^5$	−16.212	−13.603	−16.303
μKp [25, 27]	334	−2393.2	122	$7.10\cdot10^2$	−2623.8	−2528.5	−2651.5
μKd [25, 27]	364	−2413.9	128	$8.61\cdot10^2$	−2733.5	−2663.2	−2761.6
μpd [25, 28]	468	−2253.1	119	$1.11\cdot10^3$	−2859.3	−2663.2	−2884.7
μpt [25, 28]	503	−2172.6	123	$1.19\cdot10^3$	−2898.3	−2711.2	−2925.1
μdt [25, 29]	730	−1484.6	110	$1.60\cdot10^3$	−3008.1	−2711.2	−3030.4

three-particle systems considered. This is not the case for the traditional approach which may produce the unphysical positive ground state energies in the "molecular" limit, i.e. when the mass ratios of the lightest particle and the heaviest particle of the system are small.

4. Conclusions

The present work introduces a new treatment of the HO basis expansion method. Instead of only one unique size parameter in the traditional approach, the basis of the HO functions with different sizes in the Jacobi coordinates is applied. The method is based on construction of a complete set of orthogonal and translational invariant states for a given number of the HO quanta for Coulomb three-body systems of three distinguishable particles, without any approximation calculation of the non-relativistic Hamiltonian matrix elements. This ensures the convergence of the variational procedure result (an upper bound to the exact eigenvalue) as the basis is increased. In this method, we choose to calculate the two-body Hamiltonian matrix elements by means of Talmi–Moshinsky brackets. Their use greatly simplifies the derivation of expressions of the two-body Hamiltonian matrix elements and, besides that, now these brackets may be calculated by a very fast computation procedure [22]. It should be pointed out that this approach is more numerically involved than the traditional one. In this method two nonlinear variational parameters (two different oscillator lengths) in the Jacobi coordinates should be optimized instead of the only one parameter of such a type. Nevertheless, since in this method the degrees of freedom are more adapted to the physical content of the system, a better energy may be expected by solving an eigenvalue problem with a smaller dimension and, as a consequence, in less overall time it can be obtained. In fact, due to the more appropriate degrees of freedom the method may be applied to any Coulomb non-identical three-particle systems, irrespective of the masses of the particles – even for very asymmetric ones (for example, one light and two heavy particles). Another advantage of the method is that it is particularly well suited for numerical minimization with respect to nonlinear parameters, since in this method the variational energy surface was obtained to have only a global minimum and no local minima.

The efficiency of the method has been illustrated by calculation of the ground state energy for a large set of the Coulomb non-identical three-particle systems. It has been found that variational calculations of the ground state energy of these systems using the proposed method converge much faster than the traditional method with only one oscillator length. For example, in the case of zero HO excitation energy this method correctly produces the negative value of the ground state energy for all considered systems in contrast with the traditional approach, which is unable to provide the negative energy in zeroth order calculations for any of these bound systems. For very asymmetric systems (with an electron as the lightest particle) the energy of the ground state calculated in the traditional approach remains positive even up to 28 excitation HO quanta. Therefore, for systems with a molecular character the second nonlinear variational parameter is vital for a reasonable convergence.

In this method only the systems of non-identical particles are considered. Hence in these calculations nonantisymmetrized basis (8) can be used unlike the previously published method, which was devoted to the development of the HO expansion method for the Coulomb three-particle systems with two identical particles [13]. From the numerical point of view, the method for the three-particle systems with two identical particles results in more complicated expressions for matrix elements of the intrinsic Hamiltonian as in the case of non-identical particles. On the other hand, the intrinsic Hamiltonian for the system of three non-identical particles has two two-body Coulomb terms instead of only one two-body Coulomb term in the method for the three-particle systems with two identical particles. Actually, both methods are quite comparable in their convergence rate and in the computation time of the ground state energy for Coulomb three-particle systems. The formulae of the presented method do not have any underlying assumptions related to Coulomb systems. The Coulomb interaction potential may be used with virtually any two-body potential. This could greatly improve the Coulomb interaction evaluation results and considerably increase the rate of convergence of the HO basis expansion in hadronic, nuclear and molecular physics applications.

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NAUJOS HARMONINIO OSCILIATORIAUS BAZĖS TAIKYMO GALIMYBĖS SKAIČIUOJANT KULONINĖS TRIJŲ NETAPATINGŲ DALELIŲ SISTEMOS PAGRINDINĖS BŪSENOS ENERGIJĄ

A. Deveikis

Vytauto Didžiojo universitetas, Kaunas, Lietuva

Santrauka

Pasiūlytas naujas harmoninio osciliatoriaus (HO) bazės taikymo metodas skaičiuojant kuloninės trijų netapatingų dalelių sistemos nereliatyvistinę pagrindinės būsenos energiją. Skirtingai nei tradiciniuose HO bazės taikymuose, naudojančiuose tik vieną variacinį osciliatorinį parametrą, įvesti skirtingi variaciniai parametrai kiekvienai vidinei Jakobi koordinatei. Pateikto metodo veiksmingumas pademonstruotas apskaičiuojant eilės trijų netapatingų dalelių sistemų pagrindinių būsenų energijas iki 28 HO sužadinimo kvantų skaičiaus. Rezultatai palyginami su įvertinimais, gautais naudojant tradicinę HO bazę, ir kitų autorių duomenimis. Matome žymų siūlomo metodo privalumą, palyginti su tradicinio HO bazės taikymo galimybėmis, skaičiuojant kuloninių trijų netapatingų dalelių sistemų nereliatyvistines pagrindinių būsenų energijas.