Determination of the energy spectrum of a three-body Coulomb system with relativistic corrections

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On the basis of the investigation of the asymptotic behavior of the correlation functions of the corresponding field currents with the necessary quantum numbers, the analytic method for the determination of the energy spectrum of the three-body Coulomb system is suggested. Within this framework the analytical approach to determine the energy spectrum of the molecular hydrogen ions in the ground and orbital excited state is used. In our case, relativistic corrections are taken into account by the constituent mass of the constituent particles, as well as by the interaction potential. Our results show that the masses of the constituent particles differ from the masses of the particles in the free state. The increasing of the constituent mass of electron is comparatively larger than the increasing of constituent mass of the proton, deuteron, and triton. The constituent masses of the electron differ between for the molecular ions of hydrogen $^2D$, $^3D$, $^5D$, $^2T$, and $^4T$. Thus, our results on the energy spectrum of molecular hydrogen ions in the ground and excited states show good agreement with the existing results of precision spectroscopy; this is achieved by taking into account the values of the masses of constituent particles.

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I. INTRODUCTION

The energy spectrum of the bound state can be determined with a good precision within the framework of nonrelativistic quantum mechanics (NRQM) when a good selection of the potential is made. However, the nonrelativistic Schrödinger equation (SE), which gives a mathematically correct description of the bound state, is no longer sufficient since for the description of modern experimental results, obtained in both atomic [1] and hadronic physics [2], it is necessary to take into account the relativistic correction. Nevertheless, the nonrelativistic SE is the reliable tool for the bound-state energy research and its determination. In this case, real relativistic corrections are small, so the theoretical problem reduces to obtaining the relativistic corrections to the nonrelativistic interaction potential in the formalism of quantum field theory (QFT). This idea underlies the Breit potential [3] and the effective nonrelativistic quantum field theory of Caswell and Lepage [4]. Both these approaches use the scattering matrix as a source of required corrections. In the framework of quantum electrodynamics (QE) the authors of Ref. [4] studied the scattering matrix with appropriate Feynman diagrams by taking into account the renormalization and then taking the nonrelativistic limit, so they obtained the interaction potential with the relativistic corrections. Thus, the nonrelativistic QED or NRQED method for the determination of the energy spectrum by taking into account relativistic corrections was formulated. Subsequently, this method was improved in Ref. [5]. However, in these works, the relativistic corrections within the framework of the perturbation theory were taken into account mainly to the interaction potential, and the correction to the kinetic part of the interaction Hamiltonian was almost ignored. The relativistic correction to the kinetic part of the Hamiltonian in the usual quantum mechanical formalism is included only in the framework of the relativistic SE. It is known that the determination of the energy spectrum and wave functions of the bound state consisting of a few particles from the relativistic SE, from the point of view of mathematical calculations, is almost impossible. Therefore, the inclusion of the relativistic corrections into the determination of the properties of the relativistic bound state as a potential and kinetic part of the interaction Hamiltonian is one of the most urgent problems of modern theoretical study. Our work is devoted to studying this problem.

In our approach [6–8], the mass of the bound state is determined by the asymptotic behavior of the correlation function of the corresponding currents with the necessary quantum numbers. The correlation function, which is expressed in terms of the Green’s function is represented as a functional integral, which allows one to allocate the necessary asymptotic behavior, and the averaging over the external gauge field can be performed accurately. The resulting representation is similar to the Feynman functional path integral [9] in nonrelativistic quantum mechanics. In this case, the interaction potential is determined by the Feynman diagram, the resulting exchange of the gauge field, and the mass in the SE is the constituent differing from the mass of the initial state of the system, i.e., one kinetic part of the Hamiltonian is expressed in terms of the constituent mass of the constituent particles, and it differs from the initial mass state. Our results show that the difference between these masses for the light particles is essential, in particular, for the electron and for heavy particles such as an isotope of hydrogen it is not noticeable. Thus, thanks to the constituent mass of the constituent particles one can take into account relativistic corrections to the kinetic part of the interaction Hamiltonian.

The paper is organized as follows. In the second section, we briefly describe the main components for the determination of the mass spectrum of the bound states in the functional approach. In the third section we calculate the energy spectrum of the three-body Coulomb system by taking into account the one-photon exchange. In the fourth section we calculate the energies of the molecular hydrogen ions, in particular, we determine the energy spectrum of the
ground state and the calculated energy spectrum of $H_2^+$, $D_2^+$, and $T_2^+$ with the orbital excitation.

II. BOUND STATES IN THE FUNCTIONAL APPROACH

We now briefly discuss the details of our approach. Let us denote $J(x) = \Phi(x)\Phi(x)$ as the current of scalar charged particles. If we neglect the annihilation channel, then it is convenient to represent the considered correlators as the averaging over the gauge field $A_\mu(x)$ of a product of the Green’s functions $G_m(x,y|A)$ of the scalar charged particles in the external gauge field

$$\Pi(x,y) = \langle G_m(x,y|A)G_m(y,x|A)G_m(x,y|A) \rangle_A.$$  \hspace{1cm} (2.1)

The Green’s function $G_m(x,y|A)$ of the scalar charged particle in the external gauge field is defined by the equation

$$\left[i\frac{\partial}{\partial x_\mu} + \frac{g}{\sqrt{\hbar}} A_\mu(x)\right]^2 + \frac{c^2m^2}{\hbar^2} G_m(x,y|A) = \delta(x-y).$$  \hspace{1cm} (2.2)

The solution of Eq. (2.2) is represented in the functional integral form (see details in Ref. [10])

$$G_m(x,y|A) = \int_0^\infty \frac{ds}{(4\pi)^2} e^{-i(sm^2 - (x-y)^2)/4s} \int d\sigma_\beta \times \exp \left\{ig \int_0^{1} d\xi \frac{\partial}{\partial \xi} A_\mu(\xi) \right\}.$$  \hspace{1cm} (2.3)

Here the following notation is used:

$$Z_\mu(\xi) = (x-y)_\mu \xi + y_\mu - 2\sqrt{s} A_\mu(\xi);$$  \hspace{1cm} (2.4)

$$d\sigma_\beta = N\delta B_\beta \exp \left\{-\frac{1}{2} \int_0^1 d\xi B_\mu(\xi)^2 \right\}.$$

where $\sigma_\beta$ is a Gaussian measure of integration and $B_\beta$ is the variables parameterized along the “path-trajectories” and with the normalization

$$B_\beta(0) = B_\beta(1) = 0; \hspace{1cm} \int d\sigma_\beta = 1,$$

and $N$ is the normalizing constant. When averaging over the external gauge field $A_\mu(x)$ we limit ourselves to the lowest order, i.e., we take into account only the two-point Gaussian correlator

$$\left\{ \exp \left\{ i \int dx A_\mu(x)J_\mu(x) \right\} \right\}_A = \exp \left\{ -\frac{1}{2} \int dxdy J_\mu(x)D_{\alpha\beta}(x-y)J_\beta(y) \right\}.$$  \hspace{1cm} (2.5)

Here $J_\mu(x)$ is the real current, and $D_{\alpha\beta}(x-y)$ is the gauge field propagator

$$D_{\alpha\beta}(x-y) = \langle A_\alpha(x)A_\beta(y) \rangle_A = \delta_{\alpha\beta}D(x-y) + \frac{g^2}{\delta x_\alpha \delta x_\beta} D_g(x-y),$$  \hspace{1cm} (2.6)

where

$$D(x) = \int \frac{dq}{(2\pi)^2} \frac{e^{iqx}}{q^2}; \hspace{1cm} D_g(x) = \int \frac{dq}{(2\pi)^2} \frac{e^{iqx}}{q^2} \frac{d(q^2)}{q^2}.$$  \hspace{1cm} (2.7)

The bound state mass is defined as a limit

$$M = \lim_{|x| \to \infty} \frac{\ln \Pi(x-y)}{|x-y|}. \hspace{1cm} (2.8)$$

Thus, to determine the mass $M$ we have to evaluate the correlation function $\Pi(x)$ in the asymptotic limit when $|x| \to \infty$.

Substituting (2.3) into (2.1) and averaging over the external gauge field one yields

$$\Pi(x) = \langle G_{m_1}(x,y|A)G_{m_2}(y,x|A)G_{m_3}(x,y|A) \rangle_A \times \exp \left\{-\frac{|x|}{2} \left( \frac{m_1^2}{\mu_1} + \mu_1 \right) - \frac{|x|}{2} \left( \frac{m_2^2}{\mu_2} + \mu_2 \right) - \frac{|x|}{2} \left( \frac{m_3^2}{\mu_3} + \mu_3 \right) \right\}.$$  \hspace{1cm} (2.9)

Here

$$J(\mu_1,\mu_2,\mu_3) = N_1N_2N_3 \int \int \delta r_1 \delta r_2 \delta r_3 \times \exp \left\{-\frac{1}{2} \int_0^x d\tau \left[ \mu_1 \dot{r}_1^2(\tau) + \mu_2 \dot{r}_2^2(\tau) + \mu_3 \dot{r}_3^2(\tau) \right] \right\} \times \exp \left\{-W_{1,1} - W_{2,2} - W_{3,3} + \sum_{i,j=1,i\neq j}^3 W_{i,j} \right\},$$  \hspace{1cm} (2.10)

and the following notation is used:

$$W_{i,j} = \frac{q^2}{2} \left[ (1)^{i+j} \int_0^x dt_1 dt_2 Z^{(i)}(t_1)Z^{(j)}(t_2) \right].$$  \hspace{1cm} (2.11)

The representation (2.10) has the meaning of the quantum Green’s function in the Feynman functional integral form when three particles with the masses $\mu_1, \mu_2, \mu_3$ and $\mu_3$ interact via the nonlocal potential $W_{i,j}$. We emphasize that in (2.10) the functional integration is made over the four-vectors $r_1 = (r_1, r_1^4)$, $r_2 = (r_2, r_2^4)$, and $r_3 = (r_3, r_3^4)$. The term $W_{i,j}$ in this case, is defined by all kinds of Feynman diagrams. There are two types of interactions: the first is the interaction of the constituent particle via the gauge field the contribution of which is defined by the term $W_{i,j}$, the second is the interaction of the constituent particles with each other, i.e., the self-energy diagram the contribution of which is defined by the terms $W_{1,1}, W_{2,2},$ and $W_{3,3}$. In the nonrelativistic limit the terms $W_{i,j}$ correspond to the potential interactions, whereas the terms $W_{i,j}$ correspond to the nonpotential interactions, which define the renormalization mass contribution.

In the asymptotic limit $|x| \to \infty$ the integral (2.10) behaves like

$$\lim_{|x| \to \infty} J(\mu_1,\mu_2,\mu_3) = \exp \left\{-|x|E(\mu_1,\mu_2,\mu_3) \right\}.$$  \hspace{1cm} (2.12)
bound state mass is defined by the saddle point
\[ M = \frac{1}{2} \min_{\mu_1, \mu_2, \mu_3} \left\{ \frac{m_j^2}{\mu_j} + \mu_1 + \mu_2 + \mu_3 \right\}. \tag{2.13} \]

The problem is thus reduced to the evaluation of the functional integral in (2.10). This integral, however, cannot be evaluated in the general form and it is defined in various framework approaches. At present, there are no exact mathematical methods for the evaluation of this integral. Therefore, we have to apply some physical assumptions or approaches in order to somehow perform the integration over the fourth components of \( \mathbf{r}_j^{(4)} \). The integration over the four components effectively corresponds to the nonrelativistic limit. In other words, we define the interaction potential with the corrections connected with the nonperturbative, relativistic, and nonlocal characters of the interaction. In particular, if we neglect the dependence of the functional \( W_{i,j} \) in (2.11) on \( \mathbf{r}_1^{(4)} \), \( \mathbf{r}_2^{(4)} \), and \( \mathbf{r}_3^{(4)} \), then the system (2.10) is reduced to the Feynman path integral of the scalar particles with the masses \( \mu_1, \mu_2, \) and \( \mu_3 \) in NRQM [9] with the local potential. In this approximation, according to (2.10), the interaction Hamiltonian of the scalar particles with the masses \( \mu_1, \mu_2, \) and \( \mu_3 \) reads
\[ H = \frac{1}{2\mu_1} \mathbf{p}_1^2 + \frac{1}{2\mu_2} \mathbf{p}_2^2 + \frac{1}{2\mu_3} \mathbf{p}_3^2 + V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3), \tag{2.14} \]
where \( V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \) is the interaction potential which is expressed in terms of \( W_{i,j} \), then \( E(\mu_1, \mu_2, \mu_3) \) is the eigenvalue of the interaction Hamiltonian (2.14), i.e.,
\[ H \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = E(\mu_1, \mu_2, \mu_3) \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3). \tag{2.15} \]
Then, from the minimum condition of (2.13) one obtains the equation for \( \mu_j \)
\[ \mu_j - \frac{m_j^2}{\mu_j} + 2\mu_j \frac{dE(\mu_1, \mu_2, \mu_3)}{d\mu_j} = 0; \quad j = 1, 2, 3. \tag{2.16} \]
The parameters \( \mu_1, \mu_2, \) and \( \mu_3 \) have the mass dimension.

Thus, we will define the mass and the constituent mass of the bound state system with the relativistic correction. The value \( E(\mu_1, \mu_2, \mu_3) \) is defined as the eigenvalue of the interaction Hamiltonian.

In our approach, the interaction between the particles in the bound state is described by the equation (2.11), which includes all kinds of Feynman diagrams, in particular, the expressions \( W_{11}, W_{22}, W_{33} \) correspond to the self-energy diagrams, whereas \( W_{ij} (i \neq j) \) correspond to the one-photon exchange diagram in QED. The bound state energy spectrum and the wave function (WF) are defined by the SE with the constituent mass \( \mu_j \). The corrections connected with the relativistic character of the interaction are taken into account not only by the corrections to the interaction potential, but also by the parameters \( \mu_j \) (constituent mass), which are defined in (2.16). Therefore, from the SE with the constituent mass we will determine the energy spectrum of the Coulomb three-body system by taking into account the relativistic corrections.

III. GROUND-STATE ENERGY OF THE THREE-BODY COULOMB SYSTEM

In the framework of our approach, we have considered the two-body Coulomb systems [6,7] and determined the energy spectrum and WF by taking into account relativistic corrections. We now define the ground-state energy of the three-body Coulomb system with charges \( Z_1e, Z_2e, \) and \( -Z_3e \) in the framework of our approach. In this section, we will use the atomic units \( (\hbar = 1, e = 1) \). Then, the SE reads
\[ \left\{ \frac{1}{2} \sum_{j=1}^{3} \frac{\mathbf{p}_j^2}{\mu_j} + \frac{Z_1 Z_2}{|\mathbf{R}_1 - \mathbf{R}_2|} \frac{Z_1 Z_3}{|\mathbf{R}_1 - \mathbf{R}_3|} \frac{Z_2 Z_3}{|\mathbf{R}_3 - \mathbf{R}_2|} \right\} \Psi = E \Psi. \tag{3.1} \]
We introduce the Jacobi \( (\mathbf{r}_1, \mathbf{r}_2) \) and center-of-mass \( \mathbf{x} \) coordinates
\[ \mathbf{R}_1 = \mathbf{x} + \frac{\mu_3}{M} \mathbf{r}_1 + \frac{\mu_2}{M} \mathbf{r}_2; \quad \mathbf{R}_2 = \mathbf{x} + \frac{\mu_3}{M} \mathbf{r}_1 - \frac{\mu_1 + \mu_2}{M} \mathbf{r}_2; \tag{3.2} \]
where \( M = \mu_1 + \mu_2 + \mu_3 \). The SE in these variables is of the form
\[ \left\{ -\frac{1}{2\mu_{13}} \nabla^2_{\mu_{13}} - \frac{1}{2\mu_{23}} \nabla^2_{\mu_{23}} - \frac{1}{\mu_1} \left( \nabla_{\mu_1} \nabla_{\mu_1} \right) + \frac{Z_1 Z_2}{r_{12}} \right\} \Psi = E \Psi, \tag{3.3} \]
where we omitted the total kinetic energy and used the following notation:
\[ \frac{1}{\mu_{ij}} = \frac{1}{\mu_i} + \frac{1}{\mu_j}, \quad (i \neq j); \quad r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|. \tag{3.4} \]
From (3.3) we will define the energy and the WF by using the oscillator representation (OR) method [11]. The OR method is widely used for the determination of the energy levels and WF of the two-body systems. The WF, in particular, in such systems has the form
\[ \Psi(\mathbf{r}) = r^L Y_{lm}(\theta, \phi) \psi(r), \tag{3.5} \]
where \( \Psi(\mathbf{r}) \) is the radial WF. By analogy, in the three-body case we represent the WF as
\[ \Psi(\mathbf{r}_1, \mathbf{r}_2) = Y_{L_1 L_2}^{l_1 l_2} Y_{LM}^{l_1 l_2}(\mathbf{r}_1, \mathbf{r}_2) \psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_{12}). \tag{3.6} \]
Here \( \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_{12}) \) is the radial WF depending on the Hylleraas coordinates \((\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_{12}) \) [12] and the following notation is used:
\[ Y_{LM}^{l_1 l_2}(\mathbf{r}_1, \mathbf{r}_2) = \left\{ Y_{l_1}(\mathbf{r}_1) \otimes Y_{l_2}(\mathbf{r}_2) \right\}_{LM}, \tag{3.7} \]
are the solid bipolar harmonics [13] and
\[ Y_{LM}^{l_1 l_2}(\mathbf{r}_1, \mathbf{r}_2) = \mathbf{r}^{l_1 l_2}_{LM}(\mathbf{r}_1, \mathbf{r}_2) \tag{3.8} \]
are the regular solid bipolar harmonics. The actions of some operators on the regular solid bipolar harmonics are presented in Appendix A. Substituting (3.6) into (3.3) and using (A6), (A7) and (A8) and after some simplifications for (3.3) we
have
\[
\left\{-\mathcal{Y}_{LM}(\ell_1 \ell_2) \left[ \frac{1}{2 \mu_{13}} \left( \frac{\partial^2}{\partial r_1^2} + 2 + \ell_1 + \ell_2 \frac{\partial}{\partial r_1} \right) + \frac{\ell_1 + \ell_2}{r_1} \frac{\partial}{\partial r_1} + \frac{z_1 z_3}{r_1} + \frac{z_2 z_3}{r_2} - \frac{1}{r_{12}} - \frac{2}{\mu_{13} r_1} \frac{\partial^2}{\partial r_1^2} + 2 + \ell_1 + \ell_2 \frac{\partial}{\partial r_2} \right] + \frac{\ell_2 - \ell_1}{\mu_{23} r_1} \frac{\partial}{\partial r_1} + \frac{\ell_1 - \ell_2}{\mu_{12} r_1} \frac{\partial}{\partial r_1} + \frac{1}{2 \mu_{12}} \left( \frac{\partial^2}{\partial r_1^2} + 2 + \ell_1 + \ell_2 \frac{\partial}{\partial r_1} \right) + \frac{1}{r_{12}} - \frac{1}{\mu_2} r_1 \frac{\partial^2}{\partial r_1^2} + \frac{1}{r_{12}} - \frac{2}{\mu_2} r_1 \frac{\partial^2}{\partial r_1^2} \right] \right. \\
- A(\ell_1, \ell_2) \mathcal{Y}_{LM}(\ell_1 \ell_2) \left[ \frac{1}{\mu_1} \left( B(\ell_1, \ell_2) \frac{r_2}{r_{12}} \frac{\partial}{\partial r_2} + B(\ell_2, \ell_1) \frac{1}{r_{12}} \frac{\partial}{\partial r_1} + C(\ell_1, \ell_2) \right) \right. \\
- \frac{1}{\mu_1} B(\ell_1, \ell_2) \frac{r_2^2}{r_{12}} \frac{\partial}{\partial r_2} - \frac{1}{\mu_2} B(\ell_2, \ell_1) \frac{r_1^2}{r_{12}} \frac{\partial}{\partial r_1} \right] \Psi(r_1, r_2, r_{12}) = E \mathcal{Y}_{LM}(\ell_1 \ell_2) \Psi(r_1, r_2, r_{12}), \tag{3.9}
\]
where \(A(\ell_1, \ell_2), B(\ell_1, \ell_2), \) and \(C(\ell_1, \ell_2)\) are given in (A3). To get the radial SE (3.9), we multiply this equation from the left of the bipolar harmonics, and then carry out the integration over the angular variables
\[
\left\{-\mathcal{Y}_{LM}(\ell_1 \ell_2) \left[ \frac{1}{2 \mu_{13}} \left( \frac{\partial^2}{\partial r_1^2} + 2 + \ell_1 + \ell_2 \frac{\partial}{\partial r_1} \right) + \frac{\ell_1 + \ell_2}{r_1} \frac{\partial}{\partial r_1} + \frac{z_1 z_3}{r_1} + \frac{z_2 z_3}{r_2} - \frac{1}{r_{12}} - \frac{2}{\mu_{13} r_1} \frac{\partial^2}{\partial r_1^2} + 2 + \ell_1 + \ell_2 \frac{\partial}{\partial r_2} \right] + \frac{\ell_2 - \ell_1}{\mu_{23} r_1} \frac{\partial}{\partial r_1} + \frac{\ell_1 - \ell_2}{\mu_{12} r_1} \frac{\partial}{\partial r_1} + \frac{1}{2 \mu_{12}} \left( \frac{\partial^2}{\partial r_1^2} + 2 + \ell_1 + \ell_2 \frac{\partial}{\partial r_1} \right) + \frac{1}{r_{12}} - \frac{1}{\mu_2} r_1 \frac{\partial^2}{\partial r_1^2} + \frac{1}{r_{12}} - \frac{2}{\mu_2} r_1 \frac{\partial^2}{\partial r_1^2} \right] \right. \\
- W_{\ell_1+\ell_2-1}(\ell_1, \ell_1) \left( \frac{1}{\mu_1} \frac{\partial}{\partial r_1} - \frac{1}{\mu_2} \frac{\partial}{\partial r_2} \right) - W_{\ell_1+\ell_2-1}(\ell_2, \ell_1) \left( \frac{1}{\mu_1} \frac{\partial}{\partial r_1} - \frac{1}{\mu_2} \frac{\partial}{\partial r_2} \right) \right] \left[ \frac{1}{\mu_1} B(\ell_1, \ell_2) \frac{r_2}{r_{12}} \frac{\partial}{\partial r_2} + B(\ell_2, \ell_1) \frac{r_1}{r_{12}} \frac{\partial}{\partial r_1} + C(\ell_1, \ell_2) \right) \right. \\
- \frac{1}{\mu_1} B(\ell_1, \ell_2) \frac{r_2^2}{r_{12}} \frac{\partial}{\partial r_2} - \frac{1}{\mu_2} B(\ell_2, \ell_1) \frac{r_1^2}{r_{12}} \frac{\partial}{\partial r_1} \right] \Psi(r_1, r_2, r_{12}) = E \mathcal{Y}_{LM}(\ell_1 \ell_2) \Psi(r_1, r_2, r_{12}), \tag{3.10}
\]
where we used the notation
\[
W_{\ell_1 \ell_2} = \frac{I_{\ell_1 \ell_2}^{\ell_1 \ell_2}}{I_{\ell_1 \ell_2}^{\ell_1 \ell_2}}. \tag{3.11}
\]
The calculation of \(I_{\ell_1 \ell_2}^{\ell_1 \ell_2}\) for the specific values of \(\ell_i, \ell_j\) are given in Appendix B.

To determine the energy spectrum and wave functions of the radial SE (3.10), we will apply the oscillator representation (OR) method [11] for determination of eigenvalues and WF. Before determining the energy spectrum and WF of SE by means of the OR method it should be noted that this method is based on the ideas and techniques of QFT. One of the essential differences of QFT from QM is that quantized fields, which represent an assembly of an infinite number of oscillators for the ground state (or vacuum), keep their oscillatory nature in the quantum-field interaction. In the QM eigenfunctions of the most potentials differ from the Gauss behavior of the oscillatory wave function. Therefore, the variables in the original SE must be changed so that the modified equation should have solutions with the oscillator behavior at large distances. Since this transformation is not a canonical one, after the transformation we have a new system with another set of quantum numbers and wave functions, which contains, however, a subset of the original wave functions. The transformation of variables, leading to the Gaussian asymptotic behavior in the expanded space, is one of the basic elements of ORM. Let us note that a similar idea was discussed by Fock in the solution of the problem about the hydrogen spectrum using the transformation into the four-dimensionized momentum space [14]. According to the statements above, let us change the variables in the following way (for details, see [11,15]):
\[
r_1 = q_1^{2 \rho}, \quad r_2 = q_2^{2 \rho}, \quad r_{12} = q_1^{2 \rho}, \tag{3.12}
\]
where \(\rho\) is the parameter connected to the wave function behavior at large distances. After some standard simplifications for the radial SE (3.10) in the \(d\)-dimensional auxiliary space,
we obtain

\[
\begin{align*}
\left\{ \frac{1}{2\mu_3} + \frac{1}{2\mu_2} \right\} \left[ p_1^2 - \frac{2\rho(\ell_1 - \ell_2)}{q_1^2} i(q_1 P_1) \right] + \frac{1}{2\mu_3} \left[ p_2^2 - \frac{2\rho(\ell_1 - \ell_2)}{q_2^2} i(q_2 P_2) \right] \\
+ \frac{1}{2\mu_2} \left[ p_1^2 + \frac{2\rho(\ell_1 + \ell_2)}{q_2^2} i(q_1 P_2) \right] - \frac{1}{2\mu_3} \left[ q_1^{4\rho} + q_2^{4\rho} - \frac{4\rho}{4\rho_1 q_2^{4\rho}} i(q_1 P_1) i(q_2 P_2) \right] \\
- \frac{1}{2\mu_2} \left[ q_1^{4\rho} + q_2^{4\rho} - \frac{4\rho}{4\rho_1 q_2^{4\rho}} i(q_2 P_1) i(q_1 P_2) \right] - \frac{1}{2\mu_3} \left[ \ell_1 + \ell_2 \right] \left( \frac{1}{2\rho q_1^{2\rho}} i(q_1 P_1) \right) - \frac{1}{2\mu_2} \left( B(\ell_1, \ell_2) \right) \left( \frac{1}{2\rho q_1^{2\rho}} i(q_1 P_1) \right) \\
- \Phi(\ell_1, \ell_2) W_{\ell_1, \ell_2}^{\ell_1, \ell_2 - 1} \left( \frac{1}{2\rho q_1^{2\rho}} i(q_1 P_1) \right) - \frac{1}{2\mu_2} \left( B(\ell_1, \ell_2) \right) \left( \frac{1}{2\rho q_1^{2\rho}} i(q_1 P_1) \right)
\right) \Phi(q_1^2, q_2^2, q_{12}^2) = E \Phi(q_1^2, q_2^2, q_{12}^2).
\end{align*}
\]

\[(3.13)\]

Here \(d\) is the dimension of the auxiliary space: \(d = 2 + 2\rho + 2(\ell_1 + \ell_2)\). The canonical variables are expressed in the OR in terms of creation \((a^+)\) and annihilation operators \((a)\) in the space \(\mathbb{R}^d\), and then the normal ordering is carried out. Thus, the Hamiltonian can be represented as

\[H = H_0 + \varepsilon_0(E) + H_I.\]

Here \(H_0\) is the Hamiltonian of the free oscillator, \(\varepsilon_0\) is the ground-state energy in the zeroth approximation of the OR, \(H_I\) is the interaction Hamiltonian, which is also represented in the correct form by the \((a^+)\) and \((a)\) operators, and it does not contain quadratic terms of the canonical variables. The contribution of the interaction Hamiltonian is considered as a small perturbation. In quantum field theory, after the representation of the canonical variables in terms of the creation and annihilation operators and after transformation of the interaction Hamiltonian into the normal form, the requirement of the absence of the second-order field operators is equivalent, in essence, to the renormalization of the coupling constant and the WF [16–18]. Moreover, such a procedure permits one to take the main contribution into consideration in terms of the mass renormalization and in terms of the vacuum energy. In other words, all quadratic terms are completely included in the free oscillator Hamiltonian. This requirement allows formulating the following condition according to the OR:

\[\frac{\partial \varepsilon_0(E)}{\partial \omega} = 0; \quad \frac{\partial \varepsilon_0(E)}{\partial \omega_2} = 0; \quad \frac{\partial \varepsilon_0(E)}{\partial \omega_{12}} = 0,\]

\[(3.15)\]

for the purpose of finding the oscillator frequencies \(\omega_1\), \(\omega_2\), and \(\omega_{12}\), which defines the main quantum contribution. The representation of the Hamiltonian in the correct form presented in (3.11) is explained in detail in Refs. [8,15]; therefore, we give the final result for the energy spectrum in the zeroth approximation of the OR:

\[
E = \frac{\sigma^2_1}{\mu_{13}} \Gamma(d/2) [d/4 + \rho(\ell_1 - \ell_2)] + \frac{\sigma^2_2}{\mu_{23}} \Gamma(d/2) [d/4 + \rho(\ell_2 - \ell_1)] + \frac{\sigma^2_3}{\mu_{12}} \Gamma(d/2) [d/4 + \rho(\ell_1 + \ell_2)] - \frac{\Gamma(d/2) \Gamma(d/2 + 2\rho - 1)}{8\rho^2 \Gamma^2(d/2 + 2\rho - 1)} \left[ \frac{\sigma^2_1}{\mu_1^2} + \frac{\sigma^2_2}{\mu_2^2} + \frac{\sigma^2_3}{\mu_3^2} \right].
\]

\[(3.16)\]

Here, \(\sigma_1\), \(\sigma_2\), and \(\sigma_{12}\) are the parameters connected with the frequencies of the oscillator and are determined by the following system of equations, which is derived from (3.15)

\[
\begin{align*}
\frac{\sigma_1}{\mu_{13}} \Gamma(d/2) [d/4 + \rho(\ell_1 - \ell_2)] - \frac{\Gamma(d/2) \Gamma(d/2 + 2\rho)}{4\rho^2 \Gamma^2(d/2 + 2\rho - 1) \mu_{13}} Z_1Z_3 \\
\times \frac{\Gamma(d/2 + 2\rho - 1)}{\Gamma(d/2 + 2\rho - 1)} \left[ \frac{\sigma_1^2}{\mu_1^2} + \frac{\sigma_2^2}{\mu_2^2} + \frac{\sigma_3^2}{\mu_3^2} \right] = 0;
\end{align*}
\]

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The calculations of the energies of the hydrogen molecular ions of nonadiabatic calculations for H have been performed by many authors in the last decade. Moos and coworkers have done a series of similar approach has also been used by Taylor and coworkers calculated the energies and many other properties for the first-excited orbital excited state. The present study of the hydrogen molecular ions is motivated by recent projects of precise spectroscopy experiments aimed at a sup-ppb precision. Precise accuracy of the numerical calculations is ∼0.597 139 006. (4.2)

In this case, the parameters that determine the wave function are

\[ \begin{align*}
\rho &= 0.536 175; \\
\sigma_1 &= 1.220 050 167; \\
\sigma_2 &= 1.164 634 932.
\end{align*} \] (4.3)

The parameters that are associated with the WF, the accuracy of which is

\[ \begin{align*}
\delta \sigma_1 &= \delta \sigma_2 = 3.1 \times 10^{-10}; \\
\delta \sigma_{12} &= 2 \times 10^{-10}
\end{align*} \] (4.4)

are determined by numerical calculation from Eq. (3.17). The differences between the masses and the constituent masses of the proton and electron are

\[ \begin{align*}
\Delta \mu_p &= \mu_p - m_p = 0.000 298; \\
\Delta \mu_e &= \mu_e - m_e = 0.368 961 930 97.
\end{align*} \] (4.5)

Similarly, energy the of the hydrogen molecular ion D₂⁺ is calculated. In this case, the constituent mass of the deuteron and electron are

\[ \begin{align*}
\mu_d &= 3670.483 163 744 83; \\
\mu_c &= 1.369 396 577 06.
\end{align*} \] (4.6)

\[ \begin{align*}
\sigma_1, \sigma_2, \sigma_{12} \text{ being determined from (3.17), and the parameter accuracy is } \sim 10^{-10}. \]

Using the constituent mass values presented in (4.6) for the energy of the ground state of D₂⁺ from (3.16) we get

\[ E_{\text{out}} = -0.598 788 651. \] (4.7)

In this case, the parameters defining the WF are

\[ \begin{align*}
\rho &= 0.538 270 63; \\
\sigma_{12} &= 1.236 511 545; \\
\sigma_1 &= \sigma_2 = 1.175 950 073.
\end{align*} \] (4.8)

The parameters related to the wave function are also determined from Eq. (3.17) by numerical calculations, and the accuracy is as follows:

\[ \begin{align*}
\delta \sigma_1 &= \delta \sigma_2 = 3.2 \times 10^{-10}; \\
\delta \sigma_{12} &= 2.1 \times 10^{-10}.
\end{align*} \] (4.9)

The difference between the masses and constituent masses of the deuteron and electron are

\[ \begin{align*}
\Delta \mu_d &= \mu_d - m_d = 0.000 149; \\
\Delta \mu_e &= \mu_e - m_e = 0.369 396 577 06.
\end{align*} \] (4.10)
We also calculate the energy for the hydrogen molecular ion \( \text{DT}^+ \). For the values of the constituent masses, which were identified by computing
\[
\mu_t = 5496.921 \, 687 \, 435 \, 547; \quad \mu_e = 1.371 \, 797 \, 489 \, 23, \quad (4.11)
\]

\( \sigma_1, \sigma_2, \) and \( \sigma_{12} \) are determined from (3.17), and the accuracy of the numerical calculation of these parameters is \( \sim 10^{-12} \). From (3.16) by using the values of the constituent masses from (4.11) for the energy of the ground states of \( \text{T}^+ \) we have
\[
E_{\text{out}} = -0.599 \, 506 \, 967. \quad (4.12)
\]
The parameters defining the WF are
\[
\rho = 0.537 \, 095; \quad \sigma_{12} = 1.232 \, 779 \, 363; \quad \sigma_1 = \sigma_2 = 1.173 \, 880 \, 077. \quad (4.13)
\]
The parameters that are associated with the wave function, and the accuracy is as follows:
\[
\delta \sigma_1 = \delta \sigma_2 = -1.1 \times 10^{-12}; \quad \delta \sigma_{12} = 3.9 \times 10^{-12}, \quad (4.14)
\]
are determined by numerical calculation from Eq. (3.17). The difference between the masses and the constituent masses of the triton and electron are
\[
\Delta \mu_t = \mu_t - m_t = 0.0001; \quad \Delta \mu_e = \mu_e - m_e = 0.371 \, 797 \, 489 \, 23. \quad (4.15)
\]
Next, we calculate the energy for the hydrogen molecular ion \( \text{HD}^+ \). For the values of the constituent masses we have
\[
\mu_p = 1836.153 \, 021 \, 811 \, 467; \quad \mu_d = 3670.483 \, 174 \, 029 \, 692; \quad \mu_e = 1.371 \, 408 \, 740 \, 63. \quad (4.16)
\]
The parameters \( \sigma_1, \sigma_2, \) and \( \sigma_{12} \), are determined from (3.17), and the accuracy of numerical calculations is \( \sim 10^{-10} \). Using the constituent mass values presented in (4.16) for the energy of the ground state of \( \text{HD}^+ \) from (3.16) we have
\[
E_{\text{out}} = -0.597 \, 897 \, 965. \quad (4.17)
\]
The parameters defining the WF are
\[
\rho = 0.534 \, 8576; \quad \sigma_{12} = 1.216 \, 155 \, 754; \quad \sigma_1 = 1.162 \, 912 \, 969 \quad \sigma_2 = 1.161 \, 932 \, 236. \quad (4.18)
\]
Also, from Eq. (3.17) we determined the parameters connected with the WF numerical calculations and their accuracy is
\[
\delta \sigma_1 = 3.24 \times 10^{-10}; \quad \delta \sigma_2 = 3.23 \times 10^{-10}; \quad (4.19)
\]
\[
\delta \sigma_{12} = 2.13 \times 10^{-10}.
\]
The difference between the masses and the constituent masses of the proton, deuteron, and electron are
\[
\Delta \mu_p = \mu_p - m_p = 0.000 \, 32; \quad (4.20)
\]
\[
\Delta \mu_d = \mu_d - m_d = 0.000 \, 16; \quad \Delta \mu_e = \mu_e - m_e = 0.371 \, 408 \, 710 \, 63.
\]
Next, we will calculate the energy of the hydrogen molecular ion \( \text{DT}^+ \). For values of the constituent masses equal to
\[
\mu_d = 3670.483 \, 174 \, 843 \, 8164; \quad \mu_t = 5496.921 \, 687 \, 299 \, 389; \quad \mu_e = 1.228 \, 690 \, 629 \, 72, \quad (4.21)
\]
\( \sigma_1, \sigma_2, \) and \( \sigma_{12} \) are determined from (3.17), and the accuracy of the numerical calculations of these parameters is \( \sim 10^{-10} \). Using the values of the constituent masses provided in (4.21) for the ground state energy of \( \text{DT}^+ \) from (3.16) we obtain
\[
E_{\text{out}} = -0.599 \, 130 \, 678. \quad (4.22)
\]
The parameters that determine the WF are
\[
\rho = 0.536 \, 524 \, 82; \quad \sigma_{12} = 1.228 \, 690 \, 630; \quad \sigma_1 = 1.171 \, 229 \, 052; \quad \sigma_2 = 1.170 \, 898 \, 271. \quad (4.23)
\]
The parameters related to the wave function are determined from Eq. (3.17) by numerical calculations and their accuracy is
\[
\delta \sigma_1 = 3.24 \times 10^{-10}; \quad \delta \sigma_2 = 3.19 \times 10^{-10}; \quad \delta \sigma_{12} = 2.11 \times 10^{-10}. \quad (4.24)
\]
The difference between the masses and the constituent masses of the deuteron, triton, and electron are
\[
\Delta \mu_d = \mu_d - m_d = 0.000 \, 16; \quad \Delta \mu_t = \mu_t - m_t = 0.000 \, 011; \quad \Delta \mu_e = \mu_e - m_e = 0.228 \, 690 \, 629 \, 72. \quad (4.25)
\]
By analogy, we define the energy of the hydrogen molecular ion \( \text{HT}^+ \). For the values of the constituent masses, which were defined by analytic, calculation
\[
\mu_p = 1836.152 \, 905 \, 319 \, 2442; \quad \mu_d = 3670.483 \, 174 \, 029 \, 692; \quad \mu_e = 1.353 \, 605 \, 796 \, 86. \quad (4.26)
\]
The parameters \( \sigma_1, \sigma_2, \) and \( \sigma_{12} \) are determined from (3.17), and the accuracy of numerical calculations is \( \sim 10^{-10} \). Using the constituent mass values presented in (4.26) for the ground state energy of \( \text{HT}^+ \) from (3.16) we have
\[
E_{\text{out}} = -0.598 \, 176 \, 165. \quad (4.27)
\]
In this case, the parameters that determine the wave functions are
\[
\rho = 0.553 \, 8414; \quad \sigma_{12} = 1.318 \, 006 \, 676; \quad \sigma_1 = 1.228 \, 651 \, 330; \quad \sigma_2 = 1.227 \, 186 \, 927. \quad (4.28)
\]
The parameters related to the wave function are determined from Eq. (3.17) by numerical calculations, and the accuracy is as follows:
\[
\delta \sigma_1 = 2.8 \times 10^{-10}; \quad \delta \sigma_2 = 2.7 \times 10^{-10}; \quad \delta \sigma_{12} = 1.8 \times 10^{-10}. \quad (4.29)
\]
The difference between the masses and the constituent masses of the deuteron, triton, and electron are
\[
\Delta \mu_p = \mu_p - m_p = 0.000 \, 204; \quad \Delta \mu_t = \mu_t - m_t = 0.000 \, 06; \quad \Delta \mu_e = \mu_e - m_e = 0.353 \, 605 \, 767. \quad (4.30)
\]
Our results for the energy spectrum of the hydrogen molecular ions for the ground state are in good agreement with the existing results of precision spectroscopy. This agreement is achieved by taking into account the values of the masses of the constituent particles.
B. Calculation of energy spectrum of $H_2^+$, $D_2^+$, and $T_2^+$ with orbital excitation

We now proceed to the determination of the energy spectrum of the hydrogen molecular ion $H_2^+$, $D_2^+$, and $T_2^+$ with the orbital excitation. In this case, taking into account (A3) with $(\ell_1, \ell_2) = (0,1) + (1,0)$ of (3.10) after a similar simplification for the energy with the orbital excitation ($\ell = 1$) we obtain

\[
E = \frac{\omega_1^2}{8\rho^2\mu_{13}} \Gamma (2 + \rho + \ell_1 \rho) + \frac{\omega_2^2}{8\rho^2\mu_{23}} \Gamma (2 + \rho + \ell_2 \rho) + \frac{\omega_{12}^2}{8\rho^2\mu_{12}} \Gamma (3 \rho + \ell_1 \rho + \ell_2 \rho) + 2 \left( \omega_{12}^2 - \omega_1^2 - \omega_2^2 \right) \Gamma (2 \rho + \ell_1 \rho + \ell_2 \rho) + \frac{\sqrt{3}}{20} \frac{\omega_{12}^2}{\mu_{12} \rho^2} \Gamma (3 \rho + \ell_1 \rho + \ell_2 \rho) - \frac{\sqrt{3}}{20} \frac{\omega_{12}^2}{\mu_{12} \rho^2} \Gamma (3 \rho + \ell_1 \rho + \ell_2 \rho) + \left( \frac{\omega_1^2 \omega_{12}^2}{\mu_1 \omega_{12}^2} + \frac{\omega_2^2 \omega_{12}^2}{\mu_2 \omega_{12}^2} + \frac{\omega_1^2 \omega_2^2}{\mu_3 \omega_{12}^2} \right) \Gamma (5 \rho + \ell_1 \rho + \ell_2 \rho) \Gamma (1 + \rho + \ell_1 \rho + \ell_2 \rho) + \frac{8\rho^2}{8\rho^2} \Gamma^2 (3 \rho + \ell_1 \rho + \ell_2 \rho) .
\]

(4.31)

Then, using (4.31) in the OR, i.e., the conditions of the OR for the frequencies of the oscillators $\omega_1$, $\omega_2$, and $\omega_{12}$ or $(\sigma_1, \sigma_2, \text{and} \sigma_{12})$, we obtain the system of equations similar to (3.17). The details of the determination of the parameters of this system of equations are described above. Therefore, we will not dwell on analytical calculations and give the numerical values of the energy spectrum of the $P$ state.

First of all, we define the energy of the hydrogen molecular ion $H_2^+$ with the orbital excitation, the values of the constituent masses of the proton and electron are equal to

\[
\mu_p = 1836.153\,725\,347\,428; \quad \mu_e = 1.388\,824\,614\,60.
\]

(4.32)

Using the values of the constituent masses provided in (4.32), by for the energy of the orbital excited state of $H_2^+$ of (4.31) we have

\[
E_{\text{out}} = -0.596\,873\,776.
\]

(4.33)

In this case, the parameters that describe the wave functions are

\[
\rho = 0.337\,5308; \quad \sigma_{12} = 0.287\,500\,440;
\]

\[
\sigma_1 = \sigma_2 = 0.411\,604\,329.
\]

(4.34)

The difference between the masses and the masses of the constituent hydrogen molecular ion $H_2^+$ excited state with an orbital is

\[
\Delta \mu_p = \mu_p - m_p = 0.001\,024;
\]

\[
\Delta \mu_e = \mu_e - m_e = 0.388\,824\,614\,60,
\]

and accuracy

\[
\delta \sigma_1 = \delta \sigma_2 = 4.9 \times 10^{-11}; \quad \delta \sigma_{12} = 1.22 \times 10^{-12}.
\]

(4.36)

Next we define the energy of the hydrogen molecular ion $D_2^+$ with the orbital excitation, with the values of the constituent masses

\[
\mu_d = 3670.483\,038\,422\,289; \quad \mu_e = 1.723\,614\,400\,09.
\]

(4.37)

For the orbital excited state of $D_2^+$ from (4.31), by using the values provided for the constituent mass from (4.37) we have

\[
E_{\text{out}} = -0.598\,654\,879.
\]

(4.38)

In this case, the parameters defining the wave function are

\[
\rho = 0.231\,151\,05; \quad \sigma_{12} = 0.210\,495\,459;
\]

\[
\sigma_1 = \sigma_2 = 0.345\,334\,038.
\]

(4.39)

For the hydrogen molecular ion $D_2^+$ with orbital excited state the difference between the masses and constituent masses is

\[
\Delta \mu_d = \mu_d - m_d = 0.000\,024;
\]

\[
\Delta \mu_e = \mu_e - m_e = 0.723\,614\,400\,09,
\]

(4.40)

their accuracy is

\[
\delta \sigma_1 = \delta \sigma_2 = 3.45 \times 10^{-11}; \quad \delta \sigma_{12} = 4.12 \times 10^{-12}.
\]

(4.41)

Similarly, we define the energy of the hydrogen molecular ion $T_2^+$ with the orbital excitation, with the values of the constituent masses

\[
\mu_t = 5496.921\,588\,134\,978; \quad \mu_e = 1.388\,871\,313\,88.
\]

(4.42)

Also, using the values provided for the constituent mass from (4.42), for the energy of the orbital excited state of $T_2^+$ of (4.31) we have

\[
E_{\text{out}} = -0.599\,417\,102.
\]

(4.43)

In this case, the parameters defining the WF are

\[
\rho = 0.340\,349\,11; \quad \sigma_{12} = 0.291\,139\,518\,948;
\]

\[
\sigma_1 = \sigma_2 = 0.415\,490\,701\,096.
\]

(4.44)

The difference between the masses and the constituent masses for the hydrogen molecular ion $T_2^+$ with orbital excited state is

\[
\Delta \mu_t = \mu_t - m_t = 0.000\,0081;
\]

\[
\Delta \mu_e = \mu_e - m_e = 0.228\,690\,629\,72.
\]

(4.45)
and the accuracy is
\[ \delta \sigma_1 = \delta \sigma_2 = 4.83 \times 10^{-11}; \quad \delta \sigma_{12} = 1.03 \times 10^{-12}. \]  

(4.46)

Our results for the energy spectrum of the molecular hydrogen ions with the orbital excitation show good agreement with the existing results of precision spectroscopy; this is achieved by taking into account the values of the masses of the constituent particles.

V. RESULTS AND DISCUSSION

(i) The method for the analytical determination of the relativistic corrections to the kinetic part of the interaction Hamiltonian was developed. This approach defines the analytical energy spectrum of the molecular hydrogen ion in the ground and orbital excited state. The comparison of the results obtained is shown in Tables I and II as well as the values of the energy spectrum of the molecular ions of hydrogen obtained by different authors in the precision spectroscopy.

From the tables it is clear that our data are in good agreement with the precision spectroscopy results.

(ii) In our approach, the relativistic corrections are taken into account by the constituent mass of the constituent particles. Our results show that the constituent mass of the bound states is greater than the mass of the free states. An increase in the constituent mass for light particles is larger than for heavy composite particles, in particular, it is clear from (4.5), (4.10), (4.15), (4.20), (4.25), and (4.30).

(iii) From (4.5), (4.10), and (4.15) we see that the constituent mass of the electron for \( D^+_2 \) and \( T^+_2 \) increases, and the difference between the constituent masses of the proton, deuteron and triton reduces; this shows that all the relativistic effects can be accounted for only using the constituent masses of light particles, which means that in such a system light particles are more relativistic. Formula (4.35), (4.40), and (4.45) show that for the excited state the constituent mass becomes larger, it means that the excited state is more relativistic.

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APPENDIX A: ACTIONS OF SOME OPERATORS ON THE REGULAR SOLID BIPOLAR HARMONICS

First of all, we define the action of \( V_r \) on the regular solid bipolar harmonics

\[
\nabla_{r_1} \left[ \gamma^{ \ell_1 \ell_2}_{LM} (r_1, r_2) \Psi (r_1, r_2, r_{12}) \right] \left[ \nabla_{r_1} \gamma^{ \ell_1 \ell_2}_{LM} (r_1, r_2) \right] \Psi (r_1, r_2, r_{12}) + \gamma^{ \ell_1 \ell_2}_{LM} (r_1, r_2) \left\{ \frac{r_1}{r_1} \frac{\partial}{\partial r_1} + \frac{r_1 - r_2}{r_{12}} \frac{\partial}{\partial r_{12}} \right\} \Psi (r_1, r_2, r_{12}). \]  

(A1)
We also define the following actions:
\[
\nabla^2_{\ell_1} \left[ \mathcal{Y}^{\ell_1 \ell_2}_{LM}(\mathbf{r}_1, \mathbf{r}_2) \right] = \nabla^2_{\ell_2} \left[ \mathcal{Y}^{\ell_1 \ell_2}_{LM}(\mathbf{r}_1, \mathbf{r}_2) \right] = 0,
\]
\[
(\nabla_{\mathbf{r}_1} \cdot \nabla_{\mathbf{r}_2}) \mathcal{Y}^{\ell_1 \ell_2}_{LM}(\mathbf{r}_1, \mathbf{r}_2) = A(\ell_1, \ell_2) \mathcal{Y}^{\ell_1-1, \ell_2+1}_{LM}(\mathbf{r}_1, \mathbf{r}_2) + B(\ell_1, \ell_2) r_2^2 \mathcal{Y}^{\ell_1-1, \ell_2-1}_{LM}(\mathbf{r}_1, \mathbf{r}_2),
\]
\[
(\nabla_{\mathbf{r}_1} \cdot \nabla_{\mathbf{r}_2}) \mathcal{Y}^{\ell_1 \ell_2}_{LM}(\mathbf{r}_1, \mathbf{r}_2) = C(\ell_1, \ell_2) \mathcal{Y}^{\ell_1-1, \ell_2-1}_{LM}(\mathbf{r}_1, \mathbf{r}_2),
\]
\[
(\mathbf{r}_1 \cdot \nabla_{\mathbf{r}_2}) \mathcal{Y}^{\ell_1 \ell_2}_{LM}(\mathbf{r}_1, \mathbf{r}_2) = \epsilon_1 \mathcal{Y}^{\ell_1 \ell_2}_{LM}(\mathbf{r}_1, \mathbf{r}_2),
\]
where we used the notation
\[
C(\ell_1, \ell_2) = C(\ell_2, \ell_1) = (-1)^{\ell_1+\ell_2+L-1}(2\ell_1+1)(2\ell_2+1) \begin{pmatrix} \ell_1 & \ell_2 & L \\ \ell_2-1 & \ell_1-1 & 1 \end{pmatrix};
\]
\[
A(\ell_1, \ell_2) = (-1)^{\ell_1+\ell_2+L}(2\ell_1+1) \sqrt{\ell_1(\ell_1+1)} \begin{pmatrix} \ell_1 & \ell_2 & L \\ \ell_2+1 & \ell_1-1 & 1 \end{pmatrix};
\]
\[
B(\ell_1, \ell_2) = \frac{C(\ell_1, \ell_2)}{2\ell_2+1}.
\]
Using the above relations we can define the action of the Laplacians and the kinetic energy operator on the WF, which is presented in (3.9). For the functions that depend on the Hylleraas coordinates, the operator \(\nabla_{\mathbf{r}_i}\) has the form
\[
\nabla_{\mathbf{r}_i} = \frac{\mathbf{r}_1 - \mathbf{r}_2}{r_{12}} \frac{\partial}{\partial r_{12}} + \frac{\mathbf{r}_1}{r_1} \frac{\partial}{\partial r_1} + \frac{\mathbf{r}_2}{r_2} \frac{\partial}{\partial r_2}.
\]
Hence, the action of the laplacians on the radial part of the WF will look like
\[
\nabla^2_{\mathbf{r}_i} \Psi(\mathbf{r}_1, \mathbf{r}_2, r_{12}) = \left\{ \frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1} \frac{\partial}{\partial r_1} + \frac{r_2^2 + r_{12}^2 - r_1^2}{r_1 r_{12}} \frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_1} \frac{\partial}{\partial r_{12}} \right\} \Psi(\mathbf{r}_1, \mathbf{r}_2, r_{12}),
\]
\[
(\nabla_{\mathbf{r}_1} \cdot \nabla_{\mathbf{r}_2}) \Psi(\mathbf{r}_1, \mathbf{r}_2, r_{12}) = \left[ \frac{r_1^2 + r_2^2 - r_{12}^2}{2r_1 r_{12}} \frac{\partial^2}{\partial r_1 \partial r_2} - \frac{2}{r_1 r_{12}} \frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1 r_{12}} \frac{\partial}{\partial r_1} \right] \Psi(\mathbf{r}_1, \mathbf{r}_2, r_{12}).
\]
Let us present the action of the kinetic energy operator on the WF as
\[
\hat{T}[\mathcal{Y}^{\ell_1 \ell_2}_{LM} \Psi(\mathbf{r}_1, \mathbf{r}_2, r_{12})] = -[F_0 + F_1 + F_2 + F_3 + F_4],
\]
where
\[
F_0 = \mathcal{Y}^{\ell_1 \ell_2}_{LM} \left\{ \frac{1}{2\mu_{13}} \left[ \frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1} \frac{\partial}{\partial r_1} + \frac{r_2^2 + r_{12}^2 - r_1^2}{r_1 r_{12}} \frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_1} \frac{\partial}{\partial r_{12}} \right] + \frac{1}{\mu_2} \frac{r_1^2 + r_2^2 - r_{12}^2}{2r_1 r_{12}} \frac{\partial^2}{\partial r_1 \partial r_2} + \frac{1}{2\mu_{23}} \frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_1 r_{12}} \frac{\partial}{\partial r_{12}} \right\} \Psi(\mathbf{r}_1, \mathbf{r}_2, r_{12});
\]
and
\[
F_1 = \mathcal{Y}^{\ell_1 \ell_2}_{LM} \left\{ \frac{\ell_1}{\mu_{13}} \frac{\partial}{\partial r_1} + \frac{\ell_2}{\mu_2} \frac{\partial}{\partial r_2} + \frac{\ell_1}{\mu_3} \frac{\partial}{\partial r_1} + \frac{\ell_2}{\mu_3} \frac{\partial}{\partial r_1} \right\} \Psi(\mathbf{r}_1, \mathbf{r}_2, r_{12});
\]
\[
F_2 = A(\ell_1, \ell_2) \mathcal{Y}^{\ell_1-1, \ell_2+1}_{LM} \left\{ \frac{\partial}{\partial \ell_1} - \frac{\partial}{\partial \ell_2} \right\} \Psi(\mathbf{r}_1, \mathbf{r}_2, r_{12});
\]
\[
F_3 = A(\ell_2, \ell_1) \mathcal{Y}^{\ell_1+1, \ell_2-1}_{LM} \left\{ \frac{\partial}{\partial \ell_1} - \frac{\partial}{\partial \ell_2} \right\} \Psi(\mathbf{r}_1, \mathbf{r}_2, r_{12});
\]
\[
F_4 = \mathcal{Y}^{\ell_1-1, \ell_2-1}_{LM} \left\{ \frac{1}{\mu_3} \left[ B(\ell_1, \ell_2) r_2^2 \frac{\partial}{\partial \ell_2} + B(\ell_2, \ell_1) r_1^2 \frac{\partial}{\partial \ell_1} + C(\ell_1, \ell_2) \right]
- \frac{1}{\mu_1} B(\ell_1, \ell_2) r_2^2 \frac{\partial}{\partial \ell_1} - \frac{1}{\mu_2} B(\ell_2, \ell_1) r_1^2 \frac{\partial}{\partial \ell_2} \right\} \Psi(\mathbf{r}_1, \mathbf{r}_2, r_{12}),
\]
here \(\partial_j = 1/r_j(\partial/\partial r_j)\).
APPENDIX B: ANGULAR INTEGRALS EVALUATION

In our approach, the ground-state energy and the WF are determined by the radial SE. Therefore, for obtaining the radial SE one has to perform the angular integration. According to (3.6), the angular part of the WF is defined by the solid bipolar harmonics. Hence, using the actions of $\Delta$ and $\nabla$ on $Y^{LM}_{\ell_1\ell_2}(\mathbf{r}_1, \mathbf{r}_2)$ given in Appendix A, we multiply (3.9) from the left by the solid bipolar harmonics and integrate the obtained equation over the angular variables. First, we consider the integral

$$ I^{L'M'\ell'\ell'}_{LM\ell\ell}(\theta_{12}) = \int d\Omega Y^{L'M'\ell'\ell'}_{LM\ell\ell}(\mathbf{r}_1, \mathbf{r}_2)Y^{LM\ell\ell}_{L'M'\ell'\ell'}(\mathbf{r}_1, \mathbf{r}_2), \tag{B1} $$

where $\theta_{12}$ is the angle between the vectors $\mathbf{r}_1$ and $\mathbf{r}_2$, which is expressed in terms of the Hylleraas coordinates as $\cos \theta_{12} = \langle \mathbf{r}_1 \cdot \mathbf{r}_2 \rangle_{\text{H}} = \frac{r_1^2 + r_2^2 - \mathbf{r}_1 \cdot \mathbf{r}_2}{2r_1 r_2}$. This integral can be easily evaluated at certain values of quantum numbers: $L, M, \ell_1$, and $\ell_2$. In particular

$$ \{ Y_{\ell_1}(\hat{r}_1) \otimes Y_{\ell_2}(\hat{r}_2) \}_{00} = \left( \frac{-1}{4\pi} \right)^{\ell_1+\ell_2} P_{\ell_1}(\cos \theta_{12}). \tag{B2} $$

We will also use the following expressions: for bipolar harmonics we have

$$ Y_{2m} = \sqrt{4\pi} Y_{2m}^{00}, \quad Y_{2m}(\hat{r}_2) = \sqrt{4\pi} \left( \frac{r_1^2}{t_{12}} Y_{2m}^{00} + \frac{r_2^2}{t_{12}} Y_{2m}^{02} - \frac{10}{3} \frac{r_1 r_2}{t_{12}} Y_{2m}^{11} \right), \tag{B3} $$

and for the matrix elements

$$ \Pi_{a,b,\ldots,c} = \sqrt{(2a+1)(2b+1)\cdots(2c+1)}. $$

We used the following relations:

$$ \left\{ \begin{array}{l} l'_{11} \ \ L'_{11} \ \ 1 \\ l''_{11} \ \ L'_{11} \ \ 0 \\ \end{array} \right\} = \left\{ \begin{array}{l} l'_{11} \ \ L'_{11} \ \ 1 \\ l''_{11} \ \ L'_{11} \ \ 0 \\ \end{array} \right\} \frac{(-1)^{l''_{11}+l''_{11}+L}}{\sqrt{(2L'+1)(2L+1)}} \left\{ \begin{array}{l} l'_{11} \ \ L'_{11} \ \ 1 \\ l''_{11} \ \ L'_{11} \ \ 0 \\ \end{array} \right\}, \quad C^{LM}_{L-MLM} = \frac{(-1)^{L+M}}{\sqrt{2L+1}}, $$

$$ C^{00}_{l'0l'0} = (-1)^{l'_{22}} \sqrt{2L+1} \left\{ \begin{array}{l} l'_{22} \ \ 0 \\ 0 \ \ 0 \\ \end{array} \right\}, \quad C^{00}_{l''0l''0} = (-1)^{l''_{22}} \sqrt{2L'+1} \left\{ \begin{array}{l} l''_{22} \ \ 0 \\ 0 \ \ 0 \\ \end{array} \right\}. \tag{B6} $$

For the product of the two solid bipolar harmonics one has the formula

$$ \left\{ Y_{L_{1}}(\hat{r}_1) \otimes Y_{L_{2}}(\hat{r}_2) \right\}_{LM} = \sum_{L'L''} C^{LM}_{L'LM'} \sum_{\ell_1\ell_2} B^{LM}_{l_1l_2l'_1l'_2} \left\{ Y_{L_{1}}(\hat{r}_1) \otimes Y_{L_{2}}(\hat{r}_2) \right\}_{LM'}, \tag{B7} $$

where

$$ B^{LM}_{l_1l_2l'_1l'_2} = \sqrt{\frac{(2L'+1)(2L+1)(2l''_{11}+1)(2l''_{12}+1)(2L'+1)(2L+1)(4\pi)^2}{2R^4}} C^{00}_{l_1l_2l_1l_2} C^{00}_{l'_1l'_2l'_1l'_2} \left\{ \begin{array}{l} l'_{11} \ \ l'_{12} \ \ 1 \\ l''_{11} \ \ l''_{12} \ \ 0 \\ \end{array} \right\}_L \left\{ \begin{array}{l} l'_{11} \ \ l'_{12} \ \ 1 \\ l''_{11} \ \ l''_{12} \ \ 0 \\ \end{array} \right\}_L. \tag{B8} $$

Using the above relations, for certain values of the orbital quantum number, one can evaluate the angular integrals.