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Determination energy spectrum H_2^+, D_2^+ and T_2^+ molecular ions with orbital excitation

Abstract. 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. In the framework of this analytical approach we determine the energy spectrum of the molecular hydrogen ions with orbital excitation. 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 showed that the masses of the constituent particles differ from the masses of the particles in the free state. The insreasing of constituent mass of the electron is comparatively larger than the insreasing of constituent mass of the proton, deuteron and triton. Found that the constituent masses of the electron for the molecular ions of hydrogen H_2^+, D_2^+ and T_2^+ are different. Thus, our results on the energy spectrum of molecular hydrogen ions very well agreement with existing results of a precision spectroscopy, this is achieved, taking into account the value of the constituent masses of particles.
Keywords: molecular hydrogen ions, bound states in the functional approach

Introduction

The energy spectrum of the bound state can be determined with good precision in the framework of nonrelativistic quantum mechanics (NRQM) when a good selection of the potential is made. However, the nonrelativistic Schrodinger equation (SE), which gives 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 non-relativistic 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 a 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]. These both approach use the scattering matrix as a source of required corrections. The authors of [4] studied in the framework of quantum electrodynamics (QE) the scattering matrix with appropriate Feynman diagrams by taking into account renormalization and then taking the non-relativistic 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, taking into account relativistic corrections, was formulated. Subsequently, this method was improved in [5]. However, in these works, the relativistic corrections in the framework of the perturbation theory were taken into account mainly by the interaction potential, and the correction to the kinetic part the interaction Hamiltonian is almost ignored. Including the relativistic correction into the kinetic part of the Hamiltonian in the usual quantum mechanical formalism carried out only in the framework of the relativistic SE. It is known that the determination of the energy spectrum and the wave functions of the bound state consisting of few bodies 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.

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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 quantum-field Green's function is represented as a functional integral, which allows to allocate the necessary asymptotic behavior, as well as the averaging over the external gauge field can be performed accurately. The resulting representation is similar to the Feynman functional path integral [9] in non-relativistic 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 and it differs from the mass of the initial state of the system, i.e. one kinetic part of the Hamiltonian is expressed in terms of through the constituent mass of the constituent particles and it differs from the initial mass state. Our results showed that the difference between these masses for the light particles, in particular, is essential for the electron and heavy particles such as an isotope of hydrogen is not noticeable. Thus, thanks to the constituent mass of the constituent particles the allows to 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 discuss the basic details of determination a mass spectrum of the bound states in the functional approach. In Section 3, we calculate the energy spectrum of the three-body Coulomb system, taking into account the one-photon exchange. In Section 4, we calculated the energy spectrum of H_2^+, D_2^+ and T_2^+ with the orbital excitation. Appendices contain some evaluation details.

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 $A_\alpha(x)$ of a product of the Green functions $G_m(x, y \mid A)$ of the scalar charged particles in the external gauge field:

$$\Pi(x-y) = \left\langle G_{m_1}(x, y \mid A) G_{m_2}(y, x \mid A) G_{m_3}(x, y \mid A) \right\rangle_A . \tag{2.1}$$

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

$$\left[\left(i\frac{\partial}{\partial x_\alpha} + \frac{g}{c\hbar} A_\alpha(x) \right)^2 + \frac{c^2 m^2}{\hbar^2} \right] G_m(x, y \mid A) = \delta(x-y). \tag{2.2}$$

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

$$G_m(x, y \mid A) = \int_0^\infty \frac{ds}{(4s\pi)^2} \exp\left\{ -sm^2 - \frac{(x-y)^2}{4s} \right\} \int d\sigma_\beta \exp\left\{ ig \int_0^1 d\xi \frac{\partial Z_\alpha(\xi)}{\partial \xi} A_\alpha(\xi) \right\}. \tag{2.3}$$

Here the following notation is used:

$$Z_\alpha(\xi) = (x-y)_\alpha \xi + y_\alpha - 2\sqrt{s} B_\alpha(\xi);$$
$$d\sigma_\beta = N \delta B_\beta \exp\left\{ -\frac{1}{2} \int_0^1 d\xi \dot{B}^2(\xi) \right\}, \tag{2.4}$$

with the normalization

$$B_\beta(0) = B_\beta(1) = 0; \quad \int d\sigma_\beta = 1,$$

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

$$\left\langle \exp\left\{ i \int dx A_\alpha(x) J_\alpha(x) \right\} \right\rangle_A = \exp\left\{ -\frac{1}{2} \int\int dx dy J_\alpha(x) D_{\alpha\beta}(x-y) J_\beta(y) \right\}. \tag{2.5}$$

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

$$D_{\alpha\beta}(x-y)=\left\langle A_\alpha(x)A_\beta(y)\right\rangle_A=\delta_{\alpha,\beta}\quad D(x-y)+\frac{\partial^2}{\partial x_\alpha \partial y_\beta}\cdot D_d(x-y), \tag{2.6}$$

where

$$D(x)=\int\frac{dq}{(2\pi)^4}\cdot\frac{e^{iqx}}{q^2};\qquad D_d(x)=\int\frac{dq}{(2\pi)^4}\cdot\frac{e^{iqx}}{q^2}\frac{d(q^2)}{q^2}. \tag{2.7}$$

The bound state mass is defined as a limit:

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

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:

$$\begin{aligned}\Pi(x)=&\int_0^\infty\int_0^\infty\int_0^\infty\frac{d\mu_1 d\mu_2 d\mu_3}{(8\pi^2 x)^3}\cdot J(\mu_1,\mu_2,\mu_3)\times\\ &\times\exp\left\{-\frac{|x|}{2}\left(\frac{m_1^2}{\mu_1}+\mu_1\right)-\frac{|x|}{2}\left(\frac{m_2^2}{\mu_2}+\mu_2\right)-\frac{|x|}{2}\left(\frac{m_3^2}{\mu_3}+\mu_3\right)\right\}.\end{aligned} \tag{2.9}$$

Here

$$\begin{aligned}J(\mu_1,\mu_2,\mu_3)=&N_1N_2N_3\int\!\!\int\!\!\int\delta r_1\delta r_2\delta_3\times\\ &\times\exp\left\{-\frac{1}{2}\int_0^x d\tau[\mu_1\dot r_1^2(\tau)+\mu_2\dot r_2^2(\tau)+\mu_3\dot r_3^2(\tau)]\right\}\times\\ &\times\exp\left\{-W_{1,1}-W_{2,2}-W_{3,3}+2\sum_{i,j=1;i\neq j}W_{i,j}\right\},\end{aligned} \tag{2.10}$$

and the following notation is used:

$$W_{i,j}=\frac{g^2}{2}(-1)^{i+j}\int_0^x\int_0^x d\tau_1 d\tau_2 Z'^{(i)}_\alpha(\tau_1)D_{\alpha\beta}(Z^{(i)}(\tau_1)-Z^{(j)}(\tau_2))Z'^{(j)}_\beta(\tau_2). \tag{2.11}$$

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 μ_1,μ_2 and μ_3 interact via the nonlocal potential $W_{i,j}$. We emphasize that in (2.10) the functional integration is made over the four-vectors $r_1=(\vec r_1,r_1^{(4)})$, $r_2=(\vec r_2,r_2^{(4)})$ and $r_3=(\vec r_3,r_3^{(4)})$. 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 interaction the contribution of which is defined by the term $W_{i,j}(i\neq j)$; 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:

$$\lim_{|x|\to\infty}J(\mu_1,\mu_2,\mu_3)\Rightarrow\exp\{-x\cdot E(\mu_1,\mu_2,\mu_3)\}, \tag{2.12}$$

where the function $E(\mu_1,\mu_2,\mu_3)$ depends on the coupling constant g and on the μ_1,μ_2 and μ_3 parameters and does not depend on the masses m_1, m_2 and m_3. In the limit $|x|\to\infty$ the integral (2.10) is evaluated by the saddle-point method. The bound state mass is defined as follows:

$$M=\frac{1}{2}\min_{\mu_1,\mu_2,\mu_3}\left\{\frac{m_1^2}{\mu_1}+\mu_1+\frac{m_2^2}{\mu_2}+\mu_2+\frac{m_3^2}{\mu_3}+\mu_3+2E(\mu_1,\mu_2,\mu_3)\right\}. \quad (2.13)$$

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 integration over the fourth components of $r_j^{(4)}$. The integration over the fourth components effectively corresponds to the nonrelativistic limit. In other words, we define the interaction potential with the corrections connected with the non-perturbative, relativistic and nonlocal characters of the interaction. In particular, if we neglect the dependence of the functional $W_{i,j}$ in (2.11) on $r_1^{(4)}, r_2^{(4)}$ and $r_3^{(4)}$, then the system (2.10) is reduced to the Feynman path integral of the scalar particles with the masses μ_1, μ_2 and μ_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 μ_1, μ_2 and μ_3 reads:

$$H=\frac{1}{2\mu_1}\mathbf{P}_1^2+\frac{1}{2\mu_2}\mathbf{P}_2^2+\frac{1}{2\mu_3}\mathbf{P}_3^2+V(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3), \quad (2.14)$$

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 (2.10), i.e.

$$H\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=E(\mu_1,\mu_2,\mu_3)\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3). \quad (2.15)$$

Then, from the minimum condition of (2.13) one derives the equation for μ_j:

$$\mu_j-\frac{m_j^2}{\mu_j}+2\mu_j\frac{dE(\mu_1,\mu_2,\mu_3)}{d\mu_j}=0;\quad j=1,2,3. \quad (2.16)$$

The parameters μ_1, μ_2 and μ_3 have 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 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 μ_j. The corrections connected with a relativistic character of the interaction are taking into account not only by the corrections to the interaction potential, but also by the parameters μ_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 taking into account the relativistic corrections.

The calculation of the energy of the molecular hydrogen ions

In the framework of our approach we have considered two-body Coulomb systems [6,7] and determined the energy spectrum and WF 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 $(m_e=\hbar=1, e=1)$. Then, the SE reads

$$\left\{\frac{1}{2}\sum_{j=1}^{3}\frac{\vec{P}_j^2}{\mu_j}+\frac{Z_1Z_2}{|\vec{R}_1-\vec{R}_2|}-\frac{Z_1Z_3}{|\vec{R}_1-\vec{R}_3|}-\frac{Z_3Z_2}{|\vec{R}_3-\vec{R}_2|}\right\}\psi=E\psi. \quad (3.1)$$

We introduce Jacobi $(\vec{r}_1, \vec{r}_2)$ and the center-of-mass $\vec{x}$ coordinates

$$\vec{R}_1 = \vec{x} + \frac{\mu_3}{M}\vec{r}_1 + \frac{\mu_2}{M}\vec{r}_2;$$
$$\vec{R}_2 = \vec{x} + \frac{\mu_3}{M}\vec{r}_1 - \frac{\mu_1+\mu_2}{M}\vec{r}_2; \qquad (3.2)$$
$$\vec{R}_3 = \vec{x} - \frac{\mu_3+\mu_2}{M}\vec{r}_1 + \frac{\mu_2}{M}\vec{r}_2,$$

where $M = \mu_1 + \mu_2 + \mu_3$. The SE in these variables is of the form:

$$\left\{-\frac{1}{2\mu_{13}}\vec{\nabla}^2_{r_1} - \frac{1}{2\mu_{12}}\vec{\nabla}^2_{r_2} - \frac{1}{\mu_1}(\vec{\nabla}_{r_1}\vec{\nabla}_{r_2}) + \frac{Z_1Z_2}{r_{12}} - \frac{Z_1Z_3}{r_1} - \frac{Z_3Z_2}{r_2}\right\}\psi = E\psi, \qquad (3.3)$$

where we omitted the total kinetic energy term and used the following notation:

$$\frac{1}{\mu_{ij}} = \frac{1}{\mu_i} + \frac{1}{\mu_j}, (i \neq j); \quad r_{12} = |\vec{r}_1 - \vec{r}_2|. \qquad (3.4)$$

From (3.3) we will define the energy and the WF 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 this type of systems has the form:

$$\psi(\vec{r}) = r^{\ell}Y_{\ell m}(\theta,\varphi)\psi(r) \qquad (3.5)$$

where $\psi(r)$ is the radial WF. By analogy to this, in the three-body case we represent the WF as:

$$\psi(\vec{r}_1,\vec{r}_2) = r_1^{\ell_1}r_2^{\ell_2}Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2)\psi(r_1,r_2,r_{12}) \qquad (3.6)$$

Here $\psi(r_1,r_2,r_{12})$ is the radial WF depending on the Hylleraas coordinates (r_1,r_2,r_{12}) [12] and the following notation is used:

$$Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2) = \{Y_{\ell_1}(\vec{r}_1)\otimes Y_{\ell_2}(\vec{r}_2)\}_{LM} \qquad (3.7)$$

are the solid bipolar harmonics [13] and

$$Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2) = r_1^{\ell_1}r_2^{\ell_2}Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2), \qquad (3.8)$$

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) in (3.3) and using (A.6), (A.7) and (A.8) and after some simplifications for (3.3) we have:

$$\begin{aligned}
&\left\{-\mathrm{Y}_{\mathrm{LM}}^{\ell_1\ell_2}\left[\frac{1}{2\mu_{13}}\left(\frac{\partial^2}{\partial \mathrm{r}_1^2} + \frac{2+\ell_1+\ell_2}{\mathrm{r}_1}\frac{\partial}{\partial \mathrm{r}_1}\right) + \frac{\ell_1-\ell_2}{\mu_{13}\mathrm{r}_1}\frac{\partial}{\partial \mathrm{r}_1} + \frac{\mathrm{z}_1\mathrm{z}_3}{\mathrm{r}_1} + \frac{\mathrm{z}_2\mathrm{z}_3}{\mathrm{r}_2} - \frac{\mathrm{z}_1\mathrm{z}_2}{\mathrm{r}_{12}} + \right.\right.\\
&+\frac{1}{2\mu_{23}}\left(\frac{\partial^2}{\partial \mathrm{r}_2^2} + \frac{2+\ell_1+\ell_2}{\mathrm{r}_2}\frac{\partial}{\partial \mathrm{r}_2}\right) + \frac{\ell_2-\ell_1}{\mu_{23}}\frac{1}{\mathrm{r}_2}\frac{\partial}{\partial \mathrm{r}_2} + \frac{\ell_1-\ell_2}{\mu_{12}}\frac{1}{\mathrm{r}_{12}}\frac{\partial}{\partial \mathrm{r}_{12}} +\\
&+\frac{1}{2\mu_{12}}\left(\frac{\partial^2}{\partial \mathrm{r}_{12}^2} + \frac{2+\ell_1+\ell_2}{\mathrm{r}_{12}}\frac{\partial}{\partial \mathrm{r}_{12}}\right) + \frac{1}{\mu_2}\frac{\mathrm{r}_2^2+\mathrm{r}_{12}^2-\mathrm{r}_1^2}{2\mathrm{r}_2\mathrm{r}_{12}}\frac{\partial^2}{\partial \mathrm{r}_2\partial \mathrm{r}_{12}} +\\
&\left.+\frac{\ell_2-\ell_1}{2\mu_2}\frac{1}{\mathrm{r}_{12}}\frac{\partial}{\partial \mathrm{r}_{12}} + \frac{1}{\mu_3}\frac{\mathrm{r}_1^2+\mathrm{r}_2^2-\mathrm{r}_{12}^2}{2\mathrm{r}_1\mathrm{r}_2}\frac{\partial^2}{\partial \mathrm{r}_1\partial \mathrm{r}_2} + \frac{1}{\mu_1}\frac{\mathrm{r}_1^2+\mathrm{r}_{12}^2-\mathrm{r}_2^2}{2\mathrm{r}_1\mathrm{r}_2}\frac{\partial^2}{\partial \mathrm{r}_1\partial \mathrm{r}_{12}}\right] -\\
&-\mathrm{A}(\ell_1,\ell_2)\mathrm{Y}_{\mathrm{LM}}^{\ell_1-1,\ell_2+1}\left(\frac{1}{\mu_3}\frac{1}{\mathrm{r}_2}\frac{\partial}{\partial \mathrm{r}_2} - \frac{1}{\mu_1}\frac{1}{\mathrm{r}_{12}}\frac{\partial}{\partial \mathrm{r}_{12}}\right) -\\
&-\mathrm{A}(\ell_2,\ell_1)\mathrm{Y}_{\mathrm{LM}}^{\ell_1+1,\ell_2-1}\left(\frac{1}{\mu_3}\frac{1}{\mathrm{r}_1}\frac{\partial}{\partial \mathrm{r}_1} - \frac{1}{\mu_2}\frac{1}{\mathrm{r}_{12}}\frac{\partial}{\partial \mathrm{r}_{12}}\right) -\\
&-\mathrm{Y}_{\mathrm{LM}}^{\ell_1-1,\ell_2-1}\left[\frac{1}{\mu_3}\left(\mathrm{B}(\ell_1,\ell_2)\mathrm{r}_2\frac{\partial}{\partial \mathrm{r}_2} + \mathrm{B}(\ell_2,\ell_1)\mathrm{r}_1\frac{\partial}{\partial \mathrm{r}_1} + \mathrm{C}(\ell_1,\ell_2)\right) -\right.\\
&\left.\left.-\frac{1}{\mu_1}\mathrm{B}(\ell_1,\ell_2)\frac{\mathrm{r}_2^2}{\mathrm{r}_{12}}\frac{\partial}{\partial \mathrm{r}_{12}} - \frac{1}{\mu_2}\mathrm{B}(\ell_2,\ell_1)\frac{\mathrm{r}_1^2}{\mathrm{r}_{12}}\frac{\partial}{\partial \mathrm{r}_{12}}\right]\right\}\psi(\mathrm{r}_1,\mathrm{r}_2,\mathrm{r}_{12}) = \mathrm{EY}_{\mathrm{LM}}^{\ell_1,\ell_2}\psi(\mathrm{r}_1,\mathrm{r}_2,\mathrm{r}_{12}),
\end{aligned} \qquad (3.9)$$

where $A(\ell_1,\ell_2)$, $B(\ell_1,\ell_2)$ and $C(\ell_1,\ell_2)$ are given in (A.3). 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:

$$\{-\Bigg[\frac{1}{2\mu_{13}}\left(\frac{\partial^2}{\partial r_1^2}+\frac{2+\ell_1+\ell_2}{r_1}\frac{\partial}{\partial r_1}\right)+\frac{1}{2\mu_{23}}\left(\frac{\partial^2}{\partial r_2^2}+\frac{2+\ell_1+\ell_2}{r_2}\frac{\partial}{\partial r_2}\right)+$$
$$+\frac{1}{2\mu_{12}}\left(\frac{\partial^2}{\partial r_{12}^2}+\frac{2+\ell_1+\ell_2}{r_{12}}\frac{\partial}{\partial r_{12}}\right)+\frac{\ell_1-\ell_2}{\mu_{12}}\frac{1}{r_{12}}\frac{\partial}{\partial r_{12}}+\frac{\ell_1-\ell_2}{\mu_{13}}\frac{1}{r_1}\frac{\partial}{\partial r_{12}}+\frac{\ell_2-\ell_1}{2\mu_2}\frac{1}{r_{12}}\frac{\partial}{\partial r_{12}}+$$
$$\frac{1}{\mu_3}\frac{r_1^2+r_2^2-r_{12}^2}{2r_1r_2}\frac{\partial^2}{\partial r_1\partial r_2}+\frac{1}{\mu_1}\frac{r_1^2+r_{12}^2-r_2^2}{2r_1r_{12}}\frac{\partial^2}{\partial r_1\partial r_{12}}+\frac{\ell_2-\ell_1}{\mu_{23}}\frac{1}{r_2}\frac{\partial}{\partial r_2}+\frac{1}{\mu_2}\frac{r_2^2+r_{12}^2-r_2^2}{2r_2r_{12}}\frac{\partial^2}{\partial r_2\partial r_{12}}+$$
$$+\frac{z_1z_3}{r_1}+\frac{z_2z_3}{r_2}-\frac{z_1z_2}{r_{12}}\Bigg]-$$
$$-W^{\ell_1,\ell_2}_{\ell'_1-1,\ell'_2+1}A(\ell_1,\ell_2)\left(\frac{1}{\mu_3}\frac{1}{r_2}\frac{\partial}{\partial r_2}-\frac{1}{\mu_1}\frac{1}{r_{12}}\frac{\partial}{\partial r_{12}}\right)-$$
$$-W^{\ell_1,\ell_2}_{\ell'_1+1,\ell'_2-1}A(\ell_2,\ell_1)\left(\frac{1}{\mu_3}\frac{1}{r_1}\frac{\partial}{\partial r_1}-\frac{1}{\mu_2}\frac{1}{r_{12}}\frac{\partial}{\partial r_{12}}\right)-$$
$$-W^{\ell_1,\ell_2}_{\ell'_1-1,\ell'_2-1}\Bigg[\frac{1}{\mu_3}\left(B(\ell_1,\ell_2)r_2\frac{\partial}{\partial r_2}+B(\ell_2,\ell_1)r_1\frac{\partial}{\partial r_1}+C(\ell_1,\ell_2)\right)-$$
$$-\frac{1}{\mu_1}B(\ell_1,\ell_2)\frac{r_2^2}{r_{12}}\frac{\partial}{\partial r_{12}}-\frac{1}{\mu_2}B(\ell_2,\ell_1)\frac{r_1^2}{r_{12}}\frac{\partial}{\partial r_{12}}\Bigg]\Bigg\}\psi(r_1,r_2,r_{12})=E\psi(r_1,r_2,r_{12}), \qquad (3.10)$$

where we used the notation

$$W^{\ell_1,\ell_2}_{\ell'_1,\ell'_2}=\frac{I^{\ell_1,\ell_2}_{\ell''_1,\ell''_2}}{I^{\ell_1,\ell_2}_{\ell'_1,\ell'_2}}. \qquad (3.11)$$

The calculation of $I^{\ell_1,\ell_2}_{\ell'_1,\ell'_2}$ - for the specific values of ℓ_i,ℓ'_j are given in Appendix B. To determine the energy spectrum and wave functions of the radial SE (3.10) we will apply the OR method [11]. This method is based on the ideas and techniques of quantum field theory. One of the significant differences of QFT from the QM is that the quantized fields representing a set of the infinite number of oscillators for the ground state (or vacuum) remain their oscillatory nature of the quantum-field interaction. The majority of the eigenfunctions of the QM potentials differs from the Gaussian behavior of the oscillator wave function. Therefore, the variables in the source must be converted to SE so that the modified SE has the solution having the oscillatory behavior at large distances. According to the above, we perform the transformation of variables as follows (for details, see [11, 14]):

$$r_1=q_1^{2\rho},\ r_2=q_2^{2\rho},\ r_{12}=q_{12}^{2\rho}. \qquad (3.12)$$

After some standard simplifications for the radial SE (3.10) in the d – dimensional auxiliary space, we obtain:

$$\Bigg\{\frac{1}{2\mu_{13}}\frac{1}{4\rho^2q_1^{2(2\rho-1)}}\left[P_1^2-\frac{2\rho(\ell-\ell)}{q_1^2}i(q_1P_1)\right]+\frac{1}{2\mu_{23}}\frac{1}{4\rho^2q_2^{2(2\rho-1)}}\left[P_2^2-\frac{2\rho(\ell-\ell)}{q_2^2}i(q_2P_2)\right]+$$
$$+\frac{1}{2\mu_{23}}\frac{1}{4\rho^2q_2^{2(2\rho-1)}}\left[P_2^2-\frac{2\rho(\ell-\ell)}{q_2^2}i(q_2P_2)\right]+\frac{1}{2\mu_{12}}\frac{1}{4\rho^2q_2^{2(2\rho-1)}}\left[P_{12}^2-\frac{2\rho(\ell+\ell)}{q_{12}^2}i(q_{12}P_{12})\right]-$$
$$-\frac{1}{2\mu_3}\frac{q_1^{4\rho}+q_2^{4\rho}-q_{12}^{4\rho}}{4\rho^2q_1^{4\rho}q_2^{4\rho}}i(q_1P_1)i(q_2P_2)-\frac{1}{2\mu_2}\frac{q_2^{4\rho}+q_{12}^{4\rho}-q_1^{4\rho}}{4\rho^2q_2^{4\rho}q_{12}^{4\rho}}i(q_2P_2)i(q_{12}P_{12})-$$
$$-\frac{1}{2\mu_1}\frac{q_1^{4\rho}+q_{12}^{4\rho}-q_2^{4\rho}}{4\rho^2q_1^{4\rho}q_{12}^{4\rho}}i(q_1P_1)i(q_{12}P_{12})-\left(\frac{\ell}{\mu_1}+\frac{\ell}{\mu_2}\right)-\frac{1}{2\rho q_{12}^2}i(q_{12}P_{12})-\frac{z_1z_3}{q_1^{2\rho}}-\frac{z_2z_3}{q_2^{2\rho}}+\frac{z_1z_2}{q_{12}^{2\rho}}-$$

$$-A(\ell_1,\ell_2)W_{l_1,l_2}^{\ell_1-1,\ell_2+1}\left(\frac{1}{2\rho\mu_3 q_2^{4\rho}}i(q_2P_2)-\frac{1}{4\rho\mu_1 q_{12}^{4\rho}}i(q_{12}P_{12})\right)-$$

$$-A(\ell_2,\ell_1)W_{l_1,l_2}^{\ell_1+1,\ell_2-1}\left(\frac{1}{2\rho\mu_3 q_1^{4\rho}}i(q_1P_1)-\frac{1}{4\rho\mu_2 q_{12}^{4\rho}}i(q_{12}P_{12})\right)-$$

$$-W_{l_1,l_2}^{\ell_1-1,\ell_2-1}\left[\frac{1}{2\rho\mu_3}(B(\ell_1,\ell_2)i(q_2P_2)+B(\ell_2,\ell_1)i(q_1P_1)+C(\ell_1,\ell_2))-\right.$$

$$\left.-(\frac{q_2}{\mu_2}B(\ell_1,\ell_2)+\frac{q_1^{4\rho}}{\mu_2}B(\ell_2,\ell_1))\frac{1}{2\rho q_{12}^{4\rho}}i(q_{12}P_{12})\right]\Phi(q_1^2,q_2^2,q_{12}^2)=E\Phi(q_1^2,q_2^2,q_{12}^2) \tag{3.13}$$

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

$$H=H_0+\varepsilon_0(E)+H_I. \tag{3.14}$$

Here H_0 is the Hamiltonian of the free oscillator, ε_0 ground-state energy in the zeroth approximation, of the OR H_I is the interaction Hamiltonian which is also represented in the correct form of (a^+) and (a) operators, and it does not contain quadratic terms of the canonical variables. Representation of the Hamiltonian in the form presented in (3.11), explained in detail in [8] - [14], therefore, we obtain the final result for the energy spectrum with the orbital excitation $(\ell=1)$ in the zeroth approximation of the OR:

$$\begin{aligned}E=&\frac{\omega_1^{2\rho}}{8\rho^2\mu_{13}}\frac{\Gamma(2+\rho+\ell\rho)}{\Gamma(3\rho+\ell\rho)}+\frac{\omega_2^{2\rho}}{8\rho^2\mu_{23}}\frac{\Gamma(2+\rho+\ell\rho)}{\Gamma(3\rho+\ell\rho)}+\frac{\omega_{12}^{2\rho}}{8\rho^2\mu_{12}}\frac{\Gamma(2+\rho+\ell\rho)}{\Gamma(3\rho+\ell\rho)}+\\&+2(\omega_{12}^{\rho}-\omega_1^{\rho}-\omega_2^{\rho})\frac{\Gamma(2\rho+\ell\rho)}{\Gamma(3\rho+\ell\rho)}+\frac{\sqrt{3}}{20}\frac{(\omega_2^{2\rho}+\omega_1^{2\rho})}{\mu_3\rho^2}\frac{\Gamma(2+\rho+\ell\rho)}{\Gamma(3\rho+\ell\rho)}-\\&-\frac{\sqrt{3}}{20}\frac{\omega_{12}^{2\rho}}{\mu_{12}\rho^2}\frac{\Gamma(2+\rho+\ell\rho)}{\Gamma(3\rho+\ell\rho)}-\left(\frac{\omega_1^{2\rho}}{\mu_{13}}+\frac{\omega_2^{2\rho}}{\mu_{23}}+\frac{\omega_{12}^{2\rho}}{\mu_{12}}\right)\frac{\Gamma(1+\rho+\ell\rho)\Gamma(1+3\rho+\ell\rho)}{8\rho^2\Gamma^2(3\rho+\ell\rho)}+\\&+\left(\frac{\omega_1^{2\rho}\omega_2^{2\rho}}{\mu_3\omega_{12}^{2\rho}}+\frac{\omega_1^{2\rho}\omega_{12}^{2\rho}}{\mu_1\omega_2^{2\rho}}+\frac{\omega_2^{2\rho}\omega_{12}^{2\rho}}{\mu_2\omega_1^{2\rho}}\right)\frac{\Gamma(5\rho+\ell\rho)\Gamma^2(1+\rho+\ell\rho)}{8\rho^2\Gamma^2(3\rho+\ell\rho)}.\end{aligned} \tag{3.15}$$

For further calculations, we introduce the following notations:

$$\omega_1^{\rho}=\sigma_1,\ \ \omega_2^{\rho}=\sigma_2 \text{ and } \omega_{12}^{\rho}=\sigma_{12} \tag{3.16}$$

Then from the OR condition (see details in [11]), i.e. of the following system of equations:

$$\begin{cases}\dfrac{\partial E}{\partial \sigma_1}=0,\\[2mm]\dfrac{\partial E}{\partial \sigma_2}=0,\\[2mm]\dfrac{\partial E}{\partial \sigma_{12}}=0;\end{cases} \tag{3.17}$$

we determine the frequency of the oscillator, i.e. paremetrs σ_1,σ_2 and σ_{12}. These equations are evaluated numerically for a given three-body system.

Then the parameters σ_1,σ_2 and σ_{12} connected with the frequency of the oscillator and are determined by the following system of equations.

$$\frac{\sigma_1}{\mu_{13}}\cdot\frac{\Gamma(d/2)}{2\rho^2}\frac{[d/4+\rho(\ell_1-\ell_2)]}{\Gamma(d/2+2\rho-1)}-\frac{\Gamma(d/2)\Gamma(d/2+2\rho)}{4\rho^2\Gamma^2(d/2+2\rho-1)}\cdot\frac{\sigma_1}{\mu_{13}}-Z_1Z_3\times$$
$$\times\frac{\Gamma(d/2+\rho-1)}{\Gamma(d/2+2\rho-1)}-\frac{\Gamma^2(d/2)\Gamma(d/2+4\rho-1)}{4\rho^2\Gamma^3(d/2+2\rho-1)}\cdot\left[\frac{\sigma_1}{\sigma_2^2}\frac{\sigma_{12}^2}{\mu_1}-\frac{\sigma_2^2}{\sigma_1^3}\frac{\sigma_{12}^2}{\mu_2}+\frac{\sigma_1}{\sigma_{12}^2}\frac{\sigma_2^2}{\mu_3}\right]=0;$$
$$\frac{\sigma_2}{\mu_{23}}\cdot\frac{\Gamma(d/2)}{2\rho^2}\frac{[d/4+\rho(\ell_2-\ell_1)]}{\Gamma(d/2+2\rho-1)}-\frac{\Gamma(d/2)\Gamma(d/2+2\rho)}{4\rho^2\Gamma^2(d/2+2\rho-1)}\cdot\frac{\sigma_2}{\mu_{23}}-Z_2Z_3\times$$
$$\times\frac{\Gamma(d/2+\rho-1)}{\Gamma(d/2+2\rho-1)}-\frac{\Gamma^2(d/2)\Gamma(d/2+4\rho-1)}{4\rho^2\Gamma^3(d/2+2\rho-1)}\cdot\left[\frac{\sigma_2}{\sigma_1^2}\frac{\sigma_{12}^2}{\mu_2}-\frac{\sigma_1^2}{\sigma_2^3}\frac{\sigma_{12}^2}{\mu_1}+\frac{\sigma_1^2}{\sigma_{12}^2}\frac{\sigma_2}{\mu_3}\right]=0; \quad (3.18)$$
$$\frac{\sigma_{12}}{\mu_{12}}\cdot\frac{\Gamma(d/2)}{2\rho^2}\frac{[d/4-\rho(\ell_1+\ell_2)]}{\Gamma(d/2+2\rho-1)}-\frac{\Gamma(d/2)\Gamma(d/2+2\rho)}{4\rho^2\Gamma^2(d/2+2\rho-1)}\cdot\frac{\sigma_{12}}{\mu_{12}}-Z_1Z_2\times$$
$$\times\frac{\Gamma(d/2+\rho-1)}{\Gamma(d/2+2\rho-1)}-\frac{\Gamma^2(d/2)\Gamma(d/2+4\rho-1)}{4\rho^2\Gamma^3(d/2+2\rho-1)}\cdot\left[\frac{\sigma_2^2}{\sigma_1^2}\frac{\sigma_{12}}{\mu_2}-\frac{\sigma_1^2}{\sigma_2^2}\frac{\sigma_{12}}{\mu_1}+\frac{\sigma_1^2}{\sigma_{12}^3}\frac{\sigma_2}{\mu_3}\right]=0.$$

From this system of equations we define of σ_1,σ_2 and σ_{12} the parameters as a functions of the constituent masses. Further, substituting the values of these parameters into (3.15) we define the dependence of the energy spectrum of the bound states on the constituent masses of the constituent particles.

The calculation of the energy spectrum of H_2^+, D_2^+ and T_2^+ with the 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 (A.3) with $(\ell_1,\ell_2)=(0,1)+(1,0)$ of (3.10) after a similar simplification for the energy with the orbital excitation ($\ell=1$).

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 equal to:

$$\mu_p=1836.1537253474287,\quad \mu_e=1.38882461460. \quad (4.1)$$

Using the values of the constituent masses provided for the energy of the orbital excited state of H_2^+:

$$E_{our}=-0.596873776. \quad (4.2)$$

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

$$\rho=0.3375308,\quad \sigma_{12}=0.287500440,\quad \sigma_1=\sigma_2=0.411604329. \quad (4.3)$$

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

$$\Delta\mu_p=\mu_p-m_p=0.001024;\qquad \Delta\mu_e=\mu_e-m_e=0.38882461460 \quad (4.4)$$

and accuracy:

$$\delta\sigma_1=\delta\sigma_2=4.9\cdot10^{-11},\quad \delta\sigma_{12}=1.22\cdot10^{-12}. \quad (4.5)$$

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

$$\mu_d=3670.483038422289,\quad \mu_e=1.72361440009. \quad (4.6)$$

For the energy of the orbital excited state of D_2^+, using the values provided for the constituent mass from (4.6) we have:

$$E_{our}=-0.598654879. \quad (4.7)$$

In this case, the parameters defining the wave function are:

$$\rho=0.23115105,\quad \sigma_{12}=0.210495459,\quad \sigma_1=\sigma_2=0.345334038. \quad (4.8)$$

For the hydrogen molecular ion D_2^+ excited state with orbital angular difference between the masses and constituent masses are:

$$\Delta\mu_d = \mu_d - m_d = 0.000024,$$
$$\Delta\mu_e = \mu_e - m_e = 0.72361440009. \quad (4.9)$$

their accuracy is:

$$\delta\sigma_1 = \delta\sigma_2 = 3.45\cdot 10^{-11}, \quad \delta\sigma_{12} = 4.12\cdot 10^{-12}. \quad (4.10)$$

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

$$\mu_t = 5496.921588134978, \quad \mu_e = 1.38887131388. \quad (4.11)$$

Also, using the values provided for the constituent mass from (4.11), for the energy of the orbital excited state of T_2^+, we have:

$$E_{our} = -0.599417102. \quad (4.12)$$

In this case, the parameters defining the WF are:

$$\rho = 0.34034911; \quad \sigma_{12} = 0.291139518948; \quad \sigma_1 = \sigma_2 = 0.415490701096 \quad (4.13)$$

The difference between the masses and the constituent masses for the hydrogen molecular ion D_2^+ excited state with orbital are:

$$\Delta\mu_t = \mu_t - m_t = 0.0000081,$$
$$\Delta\mu_e = \mu_e - m_e = 0.22869062972 \quad (4.14)$$

accuracy:

$$\delta\sigma_1 = \delta\sigma_2 = 4.83\cdot 10^{-11}, \quad \delta\sigma_{12} = 1.03\cdot 10^{-12} \quad (4.15)$$

Author(*year*)	*Reference*	*Energy*
	H_2^+	
Taylor *et al.* (1999)	[16]	−0.596 873 738 832
Moss (1999)	[17]	−0.596 873 738 832
Zong-Chao Yan	[15]	−0.596 873 738 832
This work		−0.596 873 776
	D_2^+	
Taylor *et al.* (1999)	[16]	−0.598 654 873 220
Moss (1999)	[17]	−0.598 654 873 220
Zong-Chao Yan	[15]	−0.598 654 873 220
This work		−0.598 654 879
	T_2^+	
Zong-Chao Yan	[15]	−0.599 417 152 359
This work		−0.599 417 102

Table 1: The orbital excited state energy for the hydrogen molecular ions H_2^+, D_2^+ and T_2^+

From the *Table 1* we see, that our results for the energy spectrum of the molecular hydrogen ions with the orbital excitation good agreement with the existing results of precision spectroscopy.

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Appendix A
Actions of some operators on the regular solid bipolar harmonics

First of all, we define the action of $\vec{\nabla}_r$ on the regular solid bipolar harmonics:

$$\vec{\nabla}_{r_1}\{Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2)\cdot\psi(r_1,r_2,r_{12})\}\Big[\vec{\nabla}_{r_1}Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2)\Big]\cdot\psi(r_1,r_2,r_{12})+$$
$$+Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2)\left\{\left[\frac{\vec{r}_1}{r_1}\cdot\frac{\partial}{\partial r_1}+\frac{\vec{r}_1-\vec{r}_2}{r_{12}}\cdot\frac{\partial}{\partial r_{12}}\right]\psi(r_1,r_2,r_{12})\right\}. \tag{A.1}$$

We also define the following actions:

$$\begin{aligned}
&\vec{\nabla}_{r_1}^2\{Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2)\}=\vec{\nabla}_{r_2}^2\{Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2)\}\equiv 0,\\
&(\vec{\nabla}_{r_1}\cdot\vec{r}_2)Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2)=A(\ell_1,\ell_2)Y_{LM}^{\ell_1-1,\ell_2+1}(\vec{r}_1,\vec{r}_2)+B(\ell_1,\ell_2)r_2^2Y_{LM}^{\ell_1-1,\ell_2-1}(\vec{r}_1,\vec{r}_2),\\
&(\vec{\nabla}_{r_1}^2\cdot\vec{\nabla}_{r_2}^2)Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2)=C(\ell_1,\ell_2)Y_{LM}^{\ell_1-1,\ell_2-1}(\vec{r}_1,\vec{r}_2),\\
&(\vec{r}_1\cdot\vec{\nabla}_{r_1})Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2)=\ell_1Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2),
\end{aligned} \tag{A.2}$$

where we used the notation:

$$\begin{aligned}
&C(\ell_1,\ell_2)\equiv C(\ell_2,\ell_1)=(-1)^{\ell_1+\ell_2+L-1}(2\ell_1+1)(2\ell_2+1)\cdot\begin{Bmatrix}\ell_1 & \ell_2 & L\\ \ell_2-1 & \ell_1-1 & 1\end{Bmatrix};\\
&A(\ell_1,\ell_2)=(-1)^{\ell_1+\ell_2+L}(2\ell_1+1)\sqrt{\ell_1(\ell_2+1)}\cdot\begin{Bmatrix}\ell_1 & \ell_2 & L\\ \ell_2+1 & \ell_1-1 & 1\end{Bmatrix};\\
&B(\ell_1,\ell_2)=\frac{C(\ell_1,\ell_2)}{2\ell_2+1}.
\end{aligned} \tag{A.3}$$

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 $\vec{\nabla}_{r_1}$ has the form:

$$\vec{\nabla}_{r_1}=\frac{\vec{r}_1}{r_1}\cdot\frac{\partial}{\partial r_1}+\frac{\vec{r}_1-\vec{r}_2}{r_{12}}\cdot\frac{\partial}{\partial r_{12}}. \tag{A.4}$$

Hence, the action of the laplacians on the radial part of WF will look like:

$$\begin{aligned}
&\vec{\nabla}_{r_1}^2\psi(r_1,r_2,r_{12})=\left\{\left[\frac{\partial^2}{\partial r_1^2}+\frac{2}{r_1}\frac{\partial}{\partial r_1}\right]+\frac{r_1^2+r_{12}^2-r_2^2}{r_1r_{12}}\frac{\partial^2}{\partial r_1\partial r_{12}}+\left[\frac{\partial^2}{\partial r_{12}^2}+\frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}\right]\right\}\psi,\\
&(\vec{\nabla}_{r_1}\vec{\nabla}_{r_2})\psi(r_1,r_2,r_{12})=\left\{\frac{r_1^2+r_2^2-r_{12}^2}{2r_1r_2}\frac{\partial^2}{\partial r_1\partial r_2}-\left[\frac{\partial^2}{\partial_{12}^2}+\frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}\right]-\right.\\
&\left.-\frac{r_1^2+r_{12}^2-r_2^2}{2r_1r_{12}}\frac{\partial^2}{\partial r_1\partial r_{12}}-\frac{r_2^2+r_{12}^2-r_1^2}{2r_2r_{12}}\frac{\partial^2}{\partial r_2\partial r_{12}}\right\}\psi(r_1,r_2,r_{12}).
\end{aligned} \tag{A.5}$$

Let us present the action of the kinetic energy operator on WF as:

$$T(Y_{LM}^{\ell_1\ell_2}\cdot\psi(r_1,r_2,r_{12}))=-[F_0+F_1+F_2+F_3+F_4], \tag{A.6}$$

where

$$F_0 = Y_{LM}^{\ell_1\ell_2} \cdot \left\{ \frac{1}{2\mu_{13}} \left[\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} \right] + \frac{1}{\mu_3} \frac{r_1^2 + r_2^2 - r_{12}^2}{2r_1 r_{12}} \frac{\partial^2}{\partial r_1 \partial r_2} + \right.$$
$$+ \frac{1}{2\mu_{23}} \left[\frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2} \right] + \frac{1}{\mu_1} \frac{r_1^2 + r_{12}^2 - r_2^2}{2r_1 r_{12}} \frac{\partial^2}{\partial r_1 \partial r_{12}} + \frac{1}{\mu_2} \frac{r_2^2 + r_{12}^2 - r_1^2}{2r_2 r_{12}} \frac{\partial^2}{\partial r_2 \partial r_{12}} + \quad (A.7)$$
$$\left. + \frac{1}{2\mu_{12}} \left[\frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}} \right] \right\} \psi(r_1, r_2, r_{12}),$$

and

$$F_1 = Y_{LM}^{\ell_1\ell_2} \cdot \left\{ \frac{\ell_1 \partial_1}{\mu_{13}} + \frac{\ell_2 \partial_2}{\mu_{23}} + \left(\frac{\ell_1}{\mu_1} + \frac{\ell_2}{\mu_2} \right) \cdot \partial_{12} \right\} \psi(r_1, r_2, r_{12});$$
$$F_2 = A(\ell_1, \ell_2) \cdot Y_{LM}^{\ell_1 - 1, \ell_2 + 1} \cdot \left\{ \frac{\partial_2}{\mu_3} - \frac{\partial_{12}}{\mu_1} \right\} \psi(r_1, r_2, r_{12});$$
$$F_3 = A(\ell_2, \ell_1) \cdot Y_{LM}^{\ell_1 + 1, \ell_2 - 1} \cdot \left\{ \frac{\partial_1}{\mu_3} - \frac{\partial_{12}}{\mu_2} \right\} \psi(r_1, r_2, r_{12}); \quad (A.8)$$
$$F_4 = Y_{LM}^{\ell_1 - 1, \ell_2 - 1} \cdot \left\{ \frac{1}{\mu_3} [B(\ell_1, \ell_2) r_2^2 \partial_2 + B(\ell_2, \ell_1) r_1^2 \partial_1 + C(\ell_1, \ell_2)] - \right.$$
$$\left. - \frac{1}{\mu_1} B(\ell_1, \ell_2) r_2^2 \partial_{12} - \frac{1}{\mu_2} B(\ell_2, \ell_1) r_1^2 \partial_{12} \right\} \psi(r_1, r_2, r_{12}),$$

here $\partial_j = 1/r_j \cdot (\partial/\partial r_j)$.

Appendix B
The 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 WF is defined by the solid bipolar harmonics. Hence, using the actions of Δ and $\vec{\nabla}$ on $Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2)$ 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:

$$I_{LM\,\ell_1\ell_2}^{L'M'\ell'_1\ell'_2}(\theta_{12}) = \int d\Omega Y_{L'M'}^{\ell'_1\ell'_2}(\vec{r}_1,\vec{r}_2)\cdot Y_{LM}^{\ell_1\ell_2}(\vec{r}_1,\vec{r}_2), \tag{B.1}$$

where θ_{12} is the angle between the vectors $\vec{r}_1$ and $\vec{r}_2$ which is expressed in terms of the Hylleraas coordinates as $\cos\theta_{12} = (r_1^2 + r_2^2 - r_{12}^2)/(2r_1r_2)$. This integral can be easily evaluated at certain values of quantum numbers: L, M, ℓ_1 and ℓ_2. In particular:

$$\{Y_l(\mathbf{r}_1)\otimes Y_l(\mathbf{r}_2)\}_{00} = \frac{(-1)^l(2l+1)^{1/2}}{4\pi}P_l(\cos\theta_{12}). \tag{B.2}$$

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

$$Y_{2m} = \sqrt{4\pi}Y_{2m}^{20}, \quad Y_{2m}(\mathbf{r}_{12}) = \sqrt{4\pi}\left(\frac{r_1^2}{r_{12}^2}Y_{2m}^{20} + \frac{r_2^2}{r_{12}^2}Y_{2m}^{02} - \sqrt{\frac{10}{3}}\frac{r_1r_2}{r_{12}^2}Y_{2m}^{11}\right) \tag{B.3}$$

and for the matrix elements

$$\left\langle L'l'_1\,l'_2 \,\|\, Y_2^{20} \,\|\, L\,l_1l_2\right\rangle = (-1)^{l_1+l_2+L}\frac{\sqrt{5}}{4\pi}\Pi_{LL'l_1l_2}C_{20;l_10}^{l'_10}\begin{Bmatrix} l_1 & l_2 & L \\ L' & 2 & l'_1\end{Bmatrix}; \tag{B.4}$$

$$\left\langle L'l'_1\,l'_2 \,\|\, Y_2^{11} \,\|\, L\,l_1l_2\right\rangle = \frac{3\sqrt{5}}{4\pi}\Pi_{LL'l_1l'_2}C_{10;l_10}^{l'_10}C_{10;l_20}^{l'_20}\begin{Bmatrix} l_1 & l_2 & L \\ 1 & 1 & 2 \\ l'_1 & l'_2 & L'\end{Bmatrix}; \tag{B.5}$$

where $C_{l_1m_1;l_2m_2}^{lm}$ are the standard Clebsch-Gordan coefficients and the terms in the braces are $3j$ and $6j$ symbols, respectively. We also used the notation

$$\Pi_{a,b,\ldots,c} = \sqrt{(2a+1)(2b+1)\ldots(2c+1)}. \tag{B.6}$$

We used the following relations:

$$\begin{Bmatrix} l'_1 & l''_2 & l \\ l'_2 & l''_1 & l \\ L & L & 0\end{Bmatrix} = \frac{(-1)^{l''_1+l'_2+l+L}}{\sqrt{(2L+1)(2l+1)}}\begin{Bmatrix} l'_1 & l''_1 & l \\ l''_2 & l'_2 & L\end{Bmatrix}, \qquad C_{L-MLM}^{00} = \frac{(-1)^{L+M}}{\sqrt{2L+1}},$$

$$C_{l'_10l''_10}^{l0} = (-1)^{l'_1-l''_1}\sqrt{2l+1}\begin{pmatrix} l'_1 & l''_1 & l \\ 0 & 0 & 0\end{pmatrix}, \quad C_{l'_20l''_20}^{l0} = (-1)^{l'_2-l''_2}\sqrt{2l+1}\begin{pmatrix} l'_2 & l''_2 & l \\ 0 & 0 & 0\end{pmatrix} \tag{B.6}$$

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

$$\{Y_{l'_1}(\mathbf{r}_1)\otimes Y_{l'_2}(\mathbf{r}_2)\}_{L'M'}\{Y_{l''_1}(\mathbf{r}_1)\otimes Y_{l''_2}(\mathbf{r}_2)\}_{L''M''} = \sum_{LM} C_{L'M'L''M''}^{LM}\sum_{l_1l_2} B_{l'_1l'_2L'l''_1l''_2L''}^{l_1l_2L}\{Y_{l_1}(\mathbf{r}_1)\otimes Y_{l_2}(\mathbf{r}_2)\}_{LM} \tag{B.7}$$

where

$$B^{l_1 l_2 L}_{l_1' l_2' L' l_1'' l_2'' L''} = \sqrt{\frac{(2l_1'+1)(2l_2'+1)(2l_1''+1)(2l_2''+1)(2L'+1)(2L''+1)}{(4\pi)^2}} \times$$
$$\times C^{l_1 0}_{l_1' 0 l_1'' 0} C^{l_2 0}_{l_2' 0 l_2'' 0} \begin{Bmatrix} l_1' & l_1'' & l_1 \\ l_2' & l_2'' & l_2 \\ L' & L'' & L \end{Bmatrix}. \qquad \text{(B.8)}$$

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

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