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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 H_2^+, D_2^+, T_2^+, HD^+, DT^+, and HT^+. 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 $A_\alpha(x)$ of a product of the Green's functions $G_m(x,y|A)$ of the scalar charged particles in the external gauge field

$$\Pi(x-y) = \langle G_{m_1}(x,y|A)G_{m_2}(y,x|A)G_{m_3}(x,y|A)\rangle_A. \quad (2.1)$$

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

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

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

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

Here the following notation is used:

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

where σ_β is a Gaussian measure of integration and B_β is the variables parameterized along the "path-trajectories" and with the normalization

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

and N is the normalizing constant. When 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

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

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

$$\begin{aligned} D_{\alpha\beta}(x-y) &= \langle A_\alpha(x)A_\beta(y)\rangle_A \\ &= \delta_{\alpha,\beta}D(x-y) + \frac{\partial^2}{\partial x_\alpha\partial x_\beta}D_d(x-y), \end{aligned} \quad (2.6)$$

where

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

The bound state mass is defined as a limit

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

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

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

Here

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

and the following notation is used:

$$\begin{aligned} W_{i,j} = &\frac{g^2}{2}(-1)^{i+j}\int_0^x\int_0^x d\tau_1 d\tau_2 Z'^{(i)}{}_\alpha(\tau_1)D_{\alpha\beta} \\ &\times[Z^{(i)}(\tau_1) - Z^{(j)}(\tau_2)]Z'^{(j)}{}_\beta(\tau_2). \end{aligned} \quad (2.11)$$

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 interacts via the nonlocal potential $W_{i,j}$. We emphasize that in (2.10) the functional integration is made over the four-vectors $r_1 = (\mathbf{r}_1,r_1^{(4)})$, $r_2 = (\mathbf{r}_2,r_2^{(4)})$, and $r_3 = (\mathbf{r}_3,r_3^{(4)})$. 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 $W_{i,j},(i\neq j)$; 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 $W_{j,j}$ correspond to the nonpotential interactions, which define the renormalization mass contribution.

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

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

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 (2.9) is evaluated by the saddle-point method. The bound state mass is defined by the saddle point

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

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 $r_j^{(4)}$. 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 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 $r_1^{(4)}$, $r_2^{(4)}$, 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

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

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 μ_j

$$\mu_j-\frac{m_j^2}{\mu_j}+2\mu_j\frac{dE(\mu_1,\mu_2,\mu_3)}{d\mu_j}=0;\quad j=1,23. \tag{2.16}$$

The parameters μ_1, μ_2, and μ_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 μ_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 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 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 ($m_e=\hbar=1,e=1$). Then, the SE reads

$$\left\{\frac{1}{2}\sum_{j=1}^{3}\frac{\mathbf{P}_j^2}{\mu_j}+\frac{Z_1Z_2}{|\mathbf{R}_1-\mathbf{R}_2|}-\frac{Z_1Z_3}{|\mathbf{R}_1-\mathbf{R}_3|}-\frac{Z_3Z_2}{|\mathbf{R}_3-\mathbf{R}_2|}\right\}\Psi=E\Psi. \tag{3.1}$$

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

$$\begin{aligned}&\mathbf{R}_1=\mathbf{x}+\frac{\mu_3}{M}\mathbf{r}_1+\frac{\mu_2}{M}\mathbf{r}_2;\quad \mathbf{R}_2=\mathbf{x}+\frac{\mu_3}{M}\mathbf{r}_1-\frac{\mu_1+\mu_2}{M}\mathbf{r}_2;\\&\mathbf{R}_3=\mathbf{x}-\frac{\mu_3+\mu_2}{M}\mathbf{r}_1+\frac{\mu_2}{M}\mathbf{r}_2,\end{aligned} \tag{3.2}$$

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

$$\left\{-\frac{1}{2\mu_{13}}\nabla_{r_1}^2-\frac{1}{2\mu_{23}}\nabla_{r_2}^2-\frac{1}{\mu_1}(\boldsymbol{\nabla}_{r_1}\boldsymbol{\nabla}_{r_2})+\frac{Z_1Z_2}{r_{12}}-\frac{Z_1Z_3}{r_1}-\frac{Z_3Z_2}{r_2}\right\}\Psi=E\Psi, \tag{3.3}$$

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

$$\Psi(\mathbf{r})=r^{\ell}\mathrm{Y}_{\ell m}(\theta,\varphi)\psi(r), \tag{3.5}$$

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

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=r_1^{\ell_1}r_2^{\ell_2}\mathrm{Y}_{LM}^{\ell_1\ell_2}(\mathbf{r}_1,\mathbf{r}_2)\psi(r_1,r_2,r_{12}). \tag{3.6}$$

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:

$$\mathrm{Y}_{LM}^{\ell_1\ell_2}(\mathbf{r}_1,\mathbf{r}_2)=\left\{\mathrm{Y}_{\ell_1}(\mathbf{r}_1)\otimes\mathrm{Y}_{\ell_2}(\mathbf{r}_2)\right\}_{LM} \tag{3.7}$$

are the solid bipolar harmonics [13] and

$$\mathcal{Y}_{LM}^{\ell_1\ell_2}(\mathbf{r}_1,\mathbf{r}_2)=r_1^{\ell_1}r_2^{\ell_2}\mathrm{Y}_{LM}^{\ell_1\ell_2}(\mathbf{r}_1,\mathbf{r}_2) \tag{3.8}$$

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

$$\begin{aligned}
&\Big\{-\mathcal{Y}_{LM}^{\ell_1\ell_2}\Big[\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{\ell_1+\ell_2}{\mu_{13}r_1}\frac{\partial}{\partial r_1}+\frac{z_1z_3}{r_1}+\frac{z_2z_3}{r_2}-\frac{z_1z_2}{r_{12}}\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)\\
&\quad+\frac{\ell_2-\ell_1}{\mu_{23}r_2}\frac{\partial}{\partial r_2}+\frac{\ell_1-\ell_2}{\mu_{12}}\frac{1}{r_{12}}\frac{\partial}{\partial r_{12}}+\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{1}{\mu_2}\frac{r_1^2+r_{12}^2-r_1^2}{2r_2r_{12}}\frac{\partial^2}{\partial r_2\partial r_{12}}\\
&\quad+\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}}\Big]\\
&\quad-A\left(\ell_1,\ell_2\right)\mathcal{Y}_{LM}^{\ell_1-1,\ell_2+1}\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)-A\left(\ell_2,\ell_1\right)\mathcal{Y}_{LM}^{\ell_1+1,\ell_2-1}\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)\\
&\quad-\mathcal{Y}_{LM}^{\ell_1-1,\ell_2-1}\Big[\frac{1}{\mu_3}\left(B\left(\ell_1,\ell_2\right)r_2\frac{\partial}{\partial r_2}+B\left(\ell_2,\ell_1\right)r_1\frac{\partial}{\partial r_1}+C\left(\ell_1,\ell_2\right)\right)\\
&\quad-\frac{1}{\mu_1}B\left(\ell_1,\ell_2\right)\frac{r_2^2}{r_{12}}\frac{\partial}{\partial r_{12}}-\frac{1}{\mu_2}B\left(\ell_2,\ell_1\right)\frac{r_1^2}{r_{12}}\frac{\partial}{\partial r_{12}}\Big]\Big\}\Psi\left(r_1,r_2,r_{12}\right)=E\mathcal{Y}_{LM}^{\ell_1,\ell_2}\Psi\left(r_1,r_2,r_{12}\right), \qquad (3.9)
\end{aligned}$$

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

$$\begin{aligned}
&\Big\{-\Big[\frac{1}{2\mu_{13}}\left(\frac{\partial^2}{\partial r_1^2}+\frac{2+\ell_1+\ell_2}{r_1}\frac{\partial}{\partial r_1}\right)+\frac{1}{2\mu_{23}}\left(\frac{\partial^2}{\partial r_2^2}+\frac{2+\ell_1+\ell_2}{r_2}\frac{\partial}{\partial r_2}\right)+\frac{1}{2\mu_{12}}\left(\frac{\partial^2}{\partial r_{12}^2}+\frac{2+\ell_1+\ell_2}{r_{12}}\frac{\partial}{\partial r_{12}}\right)\\
&\quad+\frac{\ell_1-\ell_2}{2\mu_1}\frac{1}{r_{12}}\frac{\partial}{\partial r_{12}}+\frac{\ell_1-\ell_2}{\mu_{13}r_1}\frac{\partial}{\partial r_1}+\frac{\ell_2-\ell_1}{2\mu_2}\frac{1}{r_{12}}\frac{\partial}{\partial r_{12}}+\frac{1}{\mu_3}\frac{r_1^2+r_2^2-r_{12}^2}{2r_1r_2}\frac{\partial^2}{\partial r_1\partial r_2}+\frac{1}{\mu_1}\frac{r_1^2+r_{12}^2-r_2^2}{2r_1r_{12}}\frac{\partial^2}{\partial r_1\partial r_{12}}\\
&\quad+\frac{\ell_2-\ell_1}{\mu_{23}r_2}\frac{\partial}{\partial r_2}+\frac{1}{\mu_2}\frac{r_2^2+r_{12}^2-r_1^2}{2r_2r_{12}}\frac{\partial^2}{\partial r_2\partial r_{12}}+\frac{z_1z_3}{r_1}+\frac{z_2z_3}{r_2}-\frac{z_1z_2}{r_{12}}\Big]-W_{\ell_1'-1\ell_2'+1}^{\ell_1\ell_2}A\left(\ell_1,\ell_2\right)\left(\frac{1}{\mu_3}\frac{1}{r_2}\frac{\partial}{\partial r_2}-\frac{1}{\mu_1}\frac{1}{r_{12}}\frac{\partial}{\partial r_{12}}\right)\\
&\quad-W_{\ell_1'+1\ell_2'-1}^{\ell_1\ell_2}A\left(l_2,l_1\right)\left(\frac{1}{\mu_3}\frac{1}{r_1}\frac{\partial}{\partial r_1}-\frac{1}{\mu_2}\frac{1}{r_{12}}\frac{\partial}{\partial r_{12}}\right)-W_{\ell_1'-1\ell_2'-1}^{\ell_1\ell_2}\Big[\frac{1}{\mu_3}\left(B\left(\ell_1,\ell_2\right)r_2\frac{\partial}{\partial r_2}+B\left(\ell_2,\ell_1\right)r_1\frac{\partial}{\partial r_1}+C\left(\ell_1,\ell_2\right)\right)\\
&\quad-\frac{1}{\mu_1}B\left(\ell_1,\ell_2\right)\frac{r_2^2}{r_{12}}\frac{\partial}{\partial r_{12}}-\frac{1}{\mu_2}B\left(\ell_2,\ell_1\right)\frac{r_1^2}{r_{12}}\frac{\partial}{\partial r_{12}}\Big]\Big\}\Psi\left(r_1,r_2,r_{12}\right)=E\Psi\left(r_1,r_2,r_{12}\right), \qquad (3.10)
\end{aligned}$$

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 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-dimensioned momentum space [14]. According to the statements above, let us change the variables in the following way (for details, see [11,15]):

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

where ρ is the parameter connected to the wave function behaviour at large distances. After some standard simplifications for the radial SE (3.10) in the d-dimensional auxiliary space, we obtain

$$\begin{aligned}
&\Bigg\{\frac{1}{2\mu_{13}}\frac{1}{4\rho^2 q_1^{2(2\rho-1)}}\left[P_1^2-\frac{2\rho(\ell_1-\ell_2)}{q_1^2}i(q_1P_1)\right]+\frac{1}{2\mu_{23}}\frac{1}{4\rho^2 q_2^{2(2\rho-1)}}\left[P_2^2-\frac{2\rho(\ell_1-\ell_2)}{q_2^2}i(q_2P_2)\right]\\
&+\frac{1}{2\mu_{12}}\frac{1}{4\rho^2 q_2^{2(2\rho-1)}}\left[P_{12}^2+\frac{2\rho(\ell_1+\ell_2)}{q_{12}^2}i(q_{12}P_{12})\right]-\frac{1}{2\mu_3}\frac{q_1^{4\rho}+q_2^{4\rho}-q_{12}^{4\rho}}{4\rho^2 q_1^{4\rho}q_2^{4\rho}}i(q_1P_1)i(q_2P_2)\\
&-\frac{1}{2\mu_2}\frac{q_2^{4\rho}+q_{12}^{4\rho}-q_1^{4\rho}}{4\rho^2 q_2^{4\rho}q_{12}^{4\rho}}i(q_2P_2)i(q_{12}P_{12})-\frac{1}{2\mu_1}\frac{q_1^{4\rho}+q_{12}^{4\rho}-q_2^{4\rho}}{4\rho^2 q_1^{4\rho}q_{12}^{4\rho}}i(q_1P_1)i(q_{12}P_{12})\\
&-\left(\frac{\ell_1}{\mu_1}+\frac{\ell_2}{\mu_2}\right)\frac{1}{2\rho q_{12}^2}i(q_{12}P_{12})-\frac{z_1z_3}{q_1^{2\rho}}-\frac{z_2z_3}{q_2^{2\rho}}+\frac{z_1z_2}{q_{12}^{2\rho}}-A(\ell_1,\ell_2)W_{\ell'1,\ell_2'}^{\ell_1-1,\ell_2+1}\left(\frac{1}{2\rho\mu_3q_2^{4\rho}}i(q_2P_2)-\frac{1}{4\rho\mu_1q_{12}^{4\rho}}i(q_{12}P_{12})\right)\\
&-A(\ell_2,\ell_1)W_{\ell_1',\ell_2'}^{\ell_1+1,\ell_2-1}\left(\frac{1}{2\rho\mu_3q_1^{4\rho}}i(q_1P_1)-\frac{1}{4\rho\mu_2q_{12}^{4\rho}}i(q_{12}P_{12})\right)\\
&-W_{\ell_1'\ell_2'}^{\ell_1-1,\ell_2-1}\Bigg[\frac{1}{2\rho\mu_3}(B(\ell_1,\ell_2)i(q_2P_2)+B(\ell_2,\ell_1)i(q_1P_1)+C(\ell_1,\ell_2))\\
&-\left(\frac{q_2^{4\rho}}{\mu_1}B(\ell_1,\ell_2)+\frac{q_1^{4\rho}}{\mu_2}B(\ell_2,\ell_1)\right)\frac{1}{2\rho q_{12}^{4\rho}}i(q_{12}P_{12})\Bigg]\Bigg\}\Phi\big(q_1^2,q_2^2,q_{12}^2\big)=E\Phi\big(q_1^2,q_2^2,q_{12}^2\big).
\end{aligned}\tag{3.13}$$

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 (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 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 ($a^\dagger$) 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:

$$\frac{\partial\varepsilon_0(E)}{\partial\omega_1}=0;\quad\frac{\partial\varepsilon_0(E)}{\partial\omega_2}=0;\quad\frac{\partial\varepsilon_0(E)}{\partial\omega_{12}}=0,\tag{3.15}$$

for the purpose of finding the oscillator frequencies ω_1, ω_2, and ω_{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

$$\begin{aligned}
E=&\frac{\sigma_1^2}{\mu_{13}}\frac{\Gamma(d/2)}{4\rho^2}\frac{[d/4+\rho(\ell_1-\ell_2)]}{\Gamma(d/2+2\rho-1)}+\frac{\sigma_2^2}{\mu_{23}}\frac{\Gamma(d/2)}{4\rho^2}\frac{[d/4+\rho(\ell_2-\ell_1)]}{\Gamma(d/2+2\rho-1)}+\frac{\sigma_{12}^2}{\mu_{12}}\frac{\Gamma(d/2)}{4\rho^2}\frac{[d/4-\rho(\ell_1+\ell_2)]}{\Gamma(d/2+2\rho-1)}\\
&-\frac{\Gamma(d/2+\rho-1)}{\Gamma(d/2+2\rho-1)}[Z_1Z_3\sigma_1+Z_2Z_3\sigma_2-Z_1Z_2\sigma_{12}]-\frac{\Gamma^2(d/2)\Gamma(d/2+4\rho-1)}{8\rho^2\Gamma^3(d/2+2\rho-1)}\left[\frac{\sigma_1^2\sigma_{12}^2}{\sigma_2^2\mu_1}+\frac{\sigma_2^2\sigma_{12}^2}{\sigma_1^2\mu_2}+\frac{\sigma_1^2\sigma_2^2}{\sigma_{12}^2\mu_3}\right]\\
&-\frac{\Gamma(d/2)\Gamma(d/2+2\rho)}{8\rho^2\Gamma^2(d/2+2\rho-1)}\left[\frac{\sigma_1^2}{\mu_1}+\frac{\sigma_{12}^2}{\mu_1}+\frac{\sigma_2^2}{\mu_2}+\frac{\sigma_{12}^2}{\mu_2}+\frac{\sigma_2^2}{\mu_3}+\frac{\sigma_1^2}{\mu_3}\right].
\end{aligned}\tag{3.16}$$

Here, σ_1, σ_2, and σ_{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)

$$\begin{aligned}
&\frac{\sigma_1}{\mu_{13}}\frac{\Gamma(d/2)}{2\rho^2}\frac{[d/4+\rho(\ell_1-\ell_2)]}{\Gamma(d/2+2\rho-1)}-\frac{\Gamma(d/2)\Gamma(d/2+2\rho)}{4\rho^2\Gamma^2(d/2+2\rho-1)}\frac{\sigma_1}{\mu_{13}}-Z_1Z_3\\
&\times\frac{\Gamma(d/2+\rho-1)}{\Gamma(d/2+2\rho-1)}-\frac{\Gamma^2(d/2)\Gamma(d/2+4\rho-1)}{4\rho^2\Gamma^3(d/2+2\rho-1)}\left[\frac{\sigma_1\sigma_{12}^2}{\sigma_2^2\mu_1}-\frac{\sigma_2^2\sigma_{12}^2}{\sigma_1^3\mu_2}+\frac{\sigma_1\sigma_2^2}{\sigma_{12}^2\mu_3}\right]=0;
\end{aligned}$$

$$\begin{aligned}
&\frac{\sigma_2}{\mu_{23}}\frac{\Gamma(d/2)}{2\rho^2}\frac{[d/4+\rho(\ell_2-\ell_1)]}{\Gamma(d/2+2\rho-1)}-\frac{\Gamma(d/2)\Gamma(d/2+2\rho)}{4\rho^2\Gamma^2(d/2+2\rho-1)}\frac{\sigma_2}{\mu_{23}}-Z_2Z_3\\
&\quad\times\frac{\Gamma(d/2+\rho-1)}{\Gamma(d/2+2\rho-1)}-\frac{\Gamma^2(d/2)\Gamma(d/2+4\rho-1)}{4\rho^2\Gamma^3(d/2+2\rho-1)}\left[\frac{\sigma_2\sigma_{12}^2}{\sigma_1^2\mu_2}-\frac{\sigma_1^2\sigma_{12}^2}{\sigma_2^3\mu_1}+\frac{\sigma_1^2\sigma_2}{\sigma_{12}^2\mu_3}\right]=0;\\
&\frac{\sigma_{12}}{\mu_{123}}\frac{\Gamma(d/2)}{2\rho^2}\frac{[d/4-\rho(\ell_1+\ell_2)]}{\Gamma(d/2+2\rho-1)}-\frac{\Gamma(d/2)\Gamma(d/2+2\rho)}{4\rho^2\Gamma^2(d/2+2\rho-1)}\frac{\sigma_{12}}{\mu_{12}}+Z_1Z_2\\
&\quad\times\frac{\Gamma(d/2+\rho-1)}{\Gamma(d/2+2\rho-1)}-\frac{\Gamma^2(d/2)\Gamma(d/2+4\rho-1)}{4\rho^2\Gamma^3(d/2+2\rho-1)}\left[\frac{\sigma_2^2\sigma_{12}}{\sigma_1^2\mu_2}+\frac{\sigma_1^2\sigma_{12}}{\sigma_2^2\mu_1}-\frac{\sigma_1^2\sigma_2^2}{\sigma_{12}^3\mu_3}\right]=0.
\end{aligned}\tag{3.17}$$

From this system of equations we define the σ_1, σ_2, and σ_{12} parameters as functions of the constituent masses. Further, substituting the values of these parameters into (3.16) we define the dependence of the energy spectrum of the bound states on the constituent masses of the constituent particles. Then, from (2.16) we determine the constituent particle masses.

IV. CALCULATION OF ENERGY OF MOLECULAR HYDROGEN IONS

A. Determination of the energy spectrum of H_2^+, D_2^+, T_2^+, HD^+, DT^+, and HT^+ for the ground state

We now proceed to the calculations of the nonrelativistic energies of the molecular hydrogen ions for the ground and orbital excited state. The present study of the hydrogen molecular ion is motivated by recent projects of precise spectroscopy experiments [19,20] aimed at a sup-ppb precision. Precise calculations of the nonrelativistic energies of the molecular hydrogen ions were performed by many authors [21–30] in the last decade. Moos [28] and coworkers have done a series of nonadiabatic calculations for H_2^+ and its isotopes in the framework of the traditional molecular physics method. A similar approach has also been used by Taylor *et al.* [25] in their calculations of energies and polarizabilities of H_2^+ and D_2^+. Using the perimetric coordinates, Hilico and coworkers [29] calculated the energies and many other properties for H_2^+, D_2^+, and HD^+. Korobov [23,26] and Zony-Chao *et al.* [24] used variational WF in Hylleraos coordinates for the calculations of the energies of the hydrogen molecular ions H_2^+, D_2^+, T_2^+, HD^+, HT^+, and DT^+ for the ground and the first-excited P states. We use the following values of the mass of the proton, deuteron, triton, and electron [30]: $m_p = 1836.152\,701$, $m_d = 3670.483\,014$, $m_t = 5496.921\,58$ and $m_e = 1.0$. Here and below we use the atomic system of units. Also, we present the value of the nonrelativistic binding energies of the molecular ions of the hydrogen isotopes calculated by several authors [21–30].

First of all, we define the energies of the hydrogen molecular ion H_2^+. Using the values of the parameters $\mu_1 = \mu_p, \mu_2 = \mu_p$, and $\mu_3 = \mu_e$, and taking into account (3.16) and (3.17) from (2.16) we define the constituent mass of the proton and the electron

$$\mu_p = 1836.152\,999\,030\,733; \quad \mu_e = 1.368\,961\,930\,97. \tag{4.1}$$

The parameters σ_1,σ_2, and σ_{12} are determined from (3.17) and accuracy of the numerical calculations is $\sim 10^{-10}$. Using the constituent mass values presented in (4.1) for the ground state energy of H_2^+ from (3.16) we have

$$E_{\text{our}} = -0.597\,139\,006. \tag{4.2}$$

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

$$\begin{gathered}\rho = 0.536\,175; \quad \sigma_{12} = 1.220\,050\,167;\\ \sigma_1 = \sigma_2 = 1.164\,634\,932.\end{gathered}\tag{4.3}$$

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

$$\delta\sigma_1 = \delta\sigma_2 = 3.1 \times 10^{-10}; \quad \delta\sigma_{12} = 2 \times 10^{-10} \tag{4.4}$$

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

$$\begin{gathered}\Delta\mu_p = \mu_p - m_p = 0.000\,298;\\ \Delta\mu_e = \mu_e - m_e = 0.368\,961\,930\,97.\end{gathered}\tag{4.5}$$

Similarly, energy the of the hydrogen molecular ion D_2^+ is calculated. In this case, the constituent mass of the deuteron and electron are

$$\mu_d = 3670.483\,163\,744\,83; \quad \mu_e = 1.369\,396\,577\,06, \tag{4.6}$$

σ_1,σ_2, σ_{12} 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 D_2^+ from (3.16) we get

$$E_{\text{our}} = -0.598\,788\,651. \tag{4.7}$$

In this case, the parameters defining the WF are

$$\begin{gathered}\rho = 0.538\,270\,63; \quad \sigma_{12} = 1.236\,511\,545;\\ \sigma_1 = \sigma_2 = 1.175\,950\,073.\end{gathered}\tag{4.8}$$

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

$$\delta\sigma_1 = \delta\sigma_2 = 3.2 \times 10^{-10}; \quad \delta\sigma_{12} = 2.1 \times 10^{-10}. \tag{4.9}$$

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

$$\begin{gathered}\Delta\mu_d = \mu_d - m_d = 0.000\,149;\\ \Delta\mu_e = \mu_e - m_e = 0.369\,396\,577\,06.\end{gathered}\tag{4.10}$$

We also calculate the energy for the hydrogen molecular ion T_2^+. For the values of the constituent masses, which were identified by computing

$$\mu_t = 5496{,}921\,687\,435\,547; \quad \mu_e = 1{,}371\,797\,489\,23, \tag{4.11}$$

σ_1,σ_2, and σ_{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 T_2^+ we have

$$E_{\text{our}} = -0.599\,506\,967. \tag{4.12}$$

The parameters defining the WF are

$$\begin{gathered} \rho = 0.537\,095; \quad \sigma_{12} = 1.232\,779\,363; \\ \sigma_1 = \sigma_2 = 1.173\,880\,077. \end{gathered} \tag{4.13}$$

The parameters that are associated with the wave function, and the accuracy is as follows:

$$\delta\sigma_1 = \delta\sigma_2 = -1.1 \times 10^{-12}; \quad \delta\sigma_{12} = 3.9 \times 10^{-12}, \tag{4.14}$$

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

$$\begin{aligned} \Delta\mu_t &= \mu_t - m_t = 0.0001; \\ \Delta\mu_e &= \mu_e - m_e = 0.371\,797\,489\,23. \end{aligned} \tag{4.15}$$

Next, we calculate the energy for the hydrogen molecular ion HD^+. For the values of the constituent masses we have

$$\begin{gathered} \mu_p = 1836.153\,021\,811\,467; \quad \mu_d = 3670.483\,174\,029\,692; \\ \mu_e = 1.371\,408\,740\,63. \end{gathered} \tag{4.16}$$

The parameters σ_1,σ_2, and σ_{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 HD^+ from (3.16) we have

$$E_{\text{our}} = -0.597\,897\,965. \tag{4.17}$$

The parameters defining the WF are

$$\begin{gathered} \rho = 0.534\,8576; \quad \sigma_{12} = 1.216\,155\,754; \\ \sigma_1 = 1.162\,912\,969 \quad \sigma_2 = 1.161\,932\,236. \end{gathered} \tag{4.18}$$

Also, from Eq. (3.17) we determined the parameters connected with the WF numerical calculations and their accuracy is

$$\begin{gathered} \delta\sigma_1 = 3.24 \times 10^{-10}; \quad \delta\sigma_2 = 3.23 \times 10^{-10}; \\ \delta\sigma_{12} = 2.13 \times 10^{-10}. \end{gathered} \tag{4.19}$$

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

$$\begin{aligned} \Delta\mu_p &= \mu_p - m_p = 0.000\,32; \\ \Delta\mu_d &= \mu_d - m_d = 0.000\,16; \\ \Delta\mu_e &= \mu_e - m_e = 0.371\,408\,710\,63. \end{aligned} \tag{4.20}$$

Next, we will calculate the energy of the hydrogen molecular ion DT^+. For values of the constituent masses equal to

$$\begin{gathered} \mu_d = 3670.483\,174\,843\,8164; \quad \mu_t = 5496.921\,687\,299\,389; \\ \mu_e = 1.228\,690\,629\,72, \end{gathered} \tag{4.21}$$

σ_1,σ_2, and σ_{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 DT^+ from (3.16) we obtain

$$E_{\text{our}} = -0.599\,130\,678. \tag{4.22}$$

The parameters that determine the WF are

$$\begin{gathered} \rho = 0.536\,524\,82; \quad \sigma_{12} = 1.228\,690\,630; \\ \sigma_1 = 1.171\,229\,052; \quad \sigma_2 = 1.170\,898\,271. \end{gathered} \tag{4.23}$$

The parameters related to the wave function are determined from Eq. (3.17) by numerical calculations and their accuracy is

$$\begin{gathered} \delta\sigma_1 = 3.24 \times 10^{-10}; \quad \delta\sigma_2 = 3.19 \times 10^{-10}; \\ \delta\sigma_{12} = 2.11 \times 10^{-10}. \end{gathered} \tag{4.24}$$

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

$$\begin{aligned} \Delta\mu_d &= \mu_d - m_d = 0.000\,16; \\ \Delta\mu_t &= \mu_t - m_t = 0.0001; \\ \Delta\mu_e &= \mu_e - m_e = 0.228\,690\,629\,72. \end{aligned} \tag{4.25}$$

By analogy, we define the energy of the hydrogen molecular ion HT^+. For the values of the constituent masses, which were defined by analytic, calculation

$$\begin{gathered} \mu_p = 1836.152\,905\,319\,2442; \quad \mu_t = 5496.921\,648\,071\,535; \\ \mu_e = 1.353\,605\,796\,86. \end{gathered} \tag{4.26}$$

The parameters σ_1,σ_2, and σ_{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 HT^+ from (3.16) we have

$$E_{\text{our}} = -0.598\,176\,165. \tag{4.27}$$

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

$$\begin{gathered} \rho = 0.553\,8414; \quad \sigma_{12} = 1.318\,006\,676; \\ \sigma_1 = 1.228\,651\,330; \quad \sigma_2 = 1.227\,186\,927. \end{gathered} \tag{4.28}$$

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

$$\begin{gathered} \delta\sigma_1 = 2.8 \times 10^{-10}; \quad \delta\sigma_2 = 2.7 \times 10^{-10}; \\ \delta\sigma_{12} = 1.8 \times 10^{-10}. \end{gathered} \tag{4.29}$$

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

$$\begin{aligned} \Delta\mu_p &= \mu_p - m_p = 0.000\,204; \\ \Delta\mu_t &= \mu_t - m_t = 0.000\,06; \\ \Delta\mu_e &= \mu_e - m_e = 0.353\,605\,767. \end{aligned} \tag{4.30}$$

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

$$\begin{aligned} E = {} & \frac{\omega_1^{2\rho}}{8\rho^2\mu_{13}}\frac{\Gamma(2+\rho+\ell\rho)}{\Gamma(3\rho+\ell\rho)} + \frac{\omega_2^{2\rho}}{8\rho^2\mu_{23}}\frac{\Gamma(2+\rho+\ell\rho)}{\Gamma(3\rho+\ell\rho)} + \frac{\omega_{12}^{2\rho}}{8\rho^2\mu_{12}}\frac{\Gamma(2+\rho+\ell\rho)}{\Gamma(3\rho+\ell\rho)} \\ & + 2\left(\omega_{12}^{\rho} - \omega_1^{\rho} - \omega_2^{\rho}\right)\frac{\Gamma(2\rho+\ell\rho)}{\Gamma(3\rho+\ell\rho)} + \frac{\sqrt{3}}{20}\frac{\left(\omega_2^{2\rho}+\omega_1^{2\rho}\right)}{\mu_3\rho^2}\frac{\Gamma(2+\rho+\ell\rho)}{\Gamma(3\rho+\ell\rho)} \\ & - \frac{\sqrt{3}}{20}\frac{\omega_{12}^{2\rho}}{\mu_{12}\rho^2}\frac{\Gamma(2+\rho+\ell\rho)}{\Gamma(3\rho+\ell\rho)} - \left(\frac{\omega_1^{2\rho}}{\mu_{13}} + \frac{\omega_2^{2\rho}}{\mu_{23}} + \frac{\omega_{12}^{2\rho}}{\mu_{12}}\right)\frac{\Gamma(1+\rho+\ell\rho)\,\Gamma(1+3\rho+\ell\rho)}{8\rho^2\Gamma^2(3\rho+\ell\rho)} \\ & + \left(\frac{\omega_1^{2\rho}\omega_2^{2\rho}}{\mu_3\omega_{12}^{2\rho}} + \frac{\omega_1^{2\rho}\omega_{12}^{2\rho}}{\mu_1\omega_2^{2\rho}} + \frac{\omega_2^{2\rho}\omega_{12}^{2\rho}}{\mu_2\omega_1^{2\rho}}\right)\frac{\Gamma(5\rho+\ell\rho)\,\Gamma^2(1+\rho+\ell\rho)}{8\rho^2\Gamma^2(3\rho+\ell\rho)}. \end{aligned} \tag{4.31}$$

Then, using (4.31) in the OR, i.e., the conditions of the OR for the frequencies of the oscillators ω_1, ω_2 and ω_3 or (σ_1, σ_2, and σ_{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

$$\mu_p = 1836.153\,725\,347\,4287; \quad \mu_e = 1.388\,824\,614\,60. \tag{4.32}$$

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

$$E_{\text{our}} = -0.596\,873\,776. \tag{4.33}$$

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

$$\begin{gathered} \rho = 0.337\,5308; \quad \sigma_{12} = 0.287\,500\,440; \\ \sigma_1 = \sigma_2 = 0.411\,604\,329. \end{gathered} \tag{4.34}$$

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

$$\begin{aligned} \Delta\mu_p &= \mu_p - m_p = 0.001\,024; \\ \Delta\mu_e &= \mu_e - m_e = 0.388\,824\,614\,60, \end{aligned} \tag{4.35}$$

and accuracy

$$\delta\sigma_1 = \delta\sigma_2 = 4.9\times10^{-11}; \quad \delta\sigma_{12} = 1.22\times10^{-12}. \tag{4.36}$$

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

$$\mu_d = 3670.483\,038\,422\,289; \quad \mu_e = 1.723\,614\,400\,09. \tag{4.37}$$

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

$$E_{\text{our}} = -0.598\,654\,879. \tag{4.38}$$

In this case, the parameters defining the wave function are

$$\begin{gathered} \rho = 0.231\,151\,05; \quad \sigma_{12} = 0.210\,495\,459; \\ \sigma_1 = \sigma_2 = 0.345\,334\,038. \end{gathered} \tag{4.39}$$

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

$$\begin{aligned} \Delta\mu_d &= \mu_d - m_d = 0.000\,024; \\ \Delta\mu_e &= \mu_e - m_e = 0.723\,614\,400\,09, \end{aligned} \tag{4.40}$$

their accuracy is

$$\delta\sigma_1 = \delta\sigma_2 = 3.45\times10^{-11}; \quad \delta\sigma_{12} = 4.12\times10^{-12}. \tag{4.41}$$

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

$$\mu_t = 5496.921\,588\,134\,978; \quad \mu_e = 1.388\,871\,313\,88. \tag{4.42}$$

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

$$E_{\text{our}} = -0.599\,417\,102. \tag{4.43}$$

In this case, the parameters defining the WF are

$$\begin{gathered} \rho = 0.340\,349\,11; \quad \sigma_{12} = 0.291\,139\,518\,948; \\ \sigma_1 = \sigma_2 = 0{,}415\,490\,701\,096. \end{gathered} \tag{4.44}$$

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

$$\begin{aligned} \Delta\mu_t &= \mu_t - m_t = 0.000\,0081; \\ \Delta\mu_e &= \mu_e - m_e = 0.228\,690\,629\,72, \end{aligned} \tag{4.45}$$

TABLE I. The ground-state energy of the hydrogen molecular ions H_2^+, D_2^+, T_2^+, HD^+, DT^+, and HT^+. All values are given in atomic units.

Author (year)	Reference	Energy
	H_2^+	
Rebane and Filinsky (1997)	[21]	−0.597 139 063 123
Saavedra *et al.* (1998)	[22]	−0.597 139 063 123
Korobov (2000)	[23]	−0.597 139 063 123
Zong-Chao Yan (2003)	[24]	−0.597 139 063 123
This work		−0.597 139 006
	D_2^+	
Rebane and Filinsky (1997)	[21]	−0.598 788 784 33
Taylor *et al.* (1999)	[25]	−0.598 788 784 33
Korobov (2001)	[26]	−0.598 788 784 29
This work		−0.598 788 651
	T_2^+	
Frolov (2002)	[27]	−0.599 506 910 111
This work		−0.598 506 967
	HD^+	
Moss (1999)	[28]	−0.599 897 968 645
Hilico *et al.* (2000)	[29]	−0.599 897 968 644
Frolov (2002)	[27]	−0.599 897 968 645
This work		−0.599 897 965
	DT^+	
Bailey and Frolov (2002)	[30]	−0.599 130 662 855
This work		−0.599 130 678
	HT^+	
Frolov (2002)	[27]	−0.598 176 134 669
This work		−0.598 176 165

and the accuracy is

$$\delta\sigma_1 = \delta\sigma_2 = 4{,}83 \times 10^{-11}; \quad \delta\sigma_{12} = 1.03 \times 10^{-12}. \quad (4.46)$$

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.

TABLE II. The orbital excited state energy for the hydrogen molecular ions H_2^+, D_2^+, and T_2^+. All values are given in atomic units.

Author (year)	Reference	Energy
	H_2^+	
Taylor *et al.* (1999)	[25]	−0.596 873 738 832
Moss (1999)	[28]	−0.596 873 738 832
Zong-Chao Yan	[24]	−0.596 873 738 832
This work		−0.596 873 776
	D_2^+	
Taylor *et al.* (1999)	[25]	−0.598 654 873 220
Moss (1999)	[28]	−0.598 654 873 220
Zong-Chao Yan	[24]	−0.598 654 873 220
This work		−0.598 654 879
	T_2^+	
Zong-Chao Yan	[24]	−0.599 417 152 359
This work		−0.599 417 102

(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 ∇_r on the regular solid bipolar harmonics

$$\nabla_{r_1}\{\mathcal{Y}_{LM}^{\ell_1\ell_2}(\mathbf{r}_1,\mathbf{r}_2)\Psi(r_1,r_2,r_{12})\}[\nabla_{r_1}\mathcal{Y}_{LM}^{\ell_1\ell_2}(\mathbf{r}_1,\mathbf{r}_2)]\Psi(r_1,r_2,r_{12}) + \mathcal{Y}_{LM}^{\ell_1\ell_2}(\mathbf{r}_1,\mathbf{r}_2)\left\{\left[\frac{\mathbf{r}_1}{r_1}\frac{\partial}{\partial r_1} + \frac{\mathbf{r}_1-\mathbf{r}_2}{r_{12}}\frac{\partial}{\partial r_{12}}\right]\Psi(r_1,r_2,r_{12})\right\}. \quad (A1)$$

We also define the following actions:

$$\begin{aligned}
&\nabla^2_{r_1}\{\mathcal{Y}^{\ell_1\ell_2}_{LM}(\mathbf{r}_1,\mathbf{r}_2)\} = \nabla^2_{r_2}\{\mathcal{Y}^{\ell_1\ell_2}_{LM}(\mathbf{r}_1,\mathbf{r}_2)\} \equiv 0,\\
&(\boldsymbol{\nabla}_{r_1}\mathbf{r}_2)\mathcal{Y}^{\ell_1\ell_2}_{LM}(\mathbf{r}_1,\mathbf{r}_2) = A(\ell_1,\ell_2)\mathcal{Y}^{\ell_1-1,\ell_2+1}_{LM}(\mathbf{r}_1,\mathbf{r}_2) + B(\ell_1,\ell_2)r_2^2\mathcal{Y}^{\ell_1-1,\ell_2-1}_{LM}(\mathbf{r}_1,\mathbf{r}_2),\\
&(\boldsymbol{\nabla}_{r_1}\boldsymbol{\nabla}_{r_2})\mathcal{Y}^{\ell_1\ell_2}_{LM}(\mathbf{r}_1,\mathbf{r}_2) = C(\ell_1,\ell_2)\mathcal{Y}^{\ell_1-1,\ell_2-1}_{LM}(\mathbf{r}_1,\mathbf{r}_2),\\
&(\mathbf{r}_1\boldsymbol{\nabla}_{r_1})\mathcal{Y}^{\ell_1\ell_2}_{LM}(\mathbf{r}_1,\mathbf{r}_2) = \ell_1\mathcal{Y}^{\ell_1\ell_2}_{LM}(\mathbf{r}_1,\mathbf{r}_2),
\end{aligned} \tag{A2}$$

where we used the notation

$$\begin{aligned}
&C(\ell_1,\ell_2) \equiv C(\ell_2,\ell_1) = (-1)^{\ell_1+\ell_2+L-1}(2\ell_1+1)(2\ell_2+1)\begin{Bmatrix}\ell_1 & \ell_2 & L\\ \ell_2-1 & \ell_1-1 & 1\end{Bmatrix};\\
&A(\ell_1,\ell_2) = (-1)^{\ell_1+\ell_2+L}(2\ell_1+1)\sqrt{\ell_1(\ell_2+1)}\begin{Bmatrix}\ell_1 & \ell_2 & L\\ \ell_2+1 & \ell_1-1 & 1\end{Bmatrix};\\
&B(\ell_1,\ell_2) = \frac{C(\ell_1,\ell_2)}{2\ell_2+1}.
\end{aligned} \tag{A3}$$

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 $\boldsymbol{\nabla}_{r_1}$ has the form

$$\boldsymbol{\nabla}_{r_1} = \frac{\mathbf{r}_1}{r_1}\frac{\partial}{\partial r_1} + \frac{\mathbf{r}_1-\mathbf{r}_2}{r_{12}}\frac{\partial}{\partial r_{12}}. \tag{A4}$$

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

$$\begin{aligned}
\nabla^2_{r_1}\Psi(r_1,r_2,r_{12}) &= \left\{\left[\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1}\right] + \frac{r_1^2+r_{12}^2-r_2^2}{r_1r_{12}}\frac{\partial^2}{\partial r_1\partial r_{12}} + \left[\frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}\right]\right\}\Psi,\\
(\boldsymbol{\nabla}_{r_1}\boldsymbol{\nabla}_{r_2})\Psi(r_1,r_2,r_{12}) &= \left\{\frac{r_1^2+r_2^2-r_{12}^2}{2r_1r_2}\frac{\partial^2}{\partial r_1\partial r_2} - \left[\frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}\right]\right.\\
&\quad\left. - \frac{r_1^2+r_{12}^2-r_2^2}{2r_1r_{12}}\frac{\partial^2}{\partial r_1\partial r_{12}} - \frac{r_2^2+r_{12}^2-r_2^1}{2r_2r_{12}}\frac{\partial^2}{\partial r_2\partial r_{12}}\right\}\Psi(r_1,r_2,r_{12}).
\end{aligned} \tag{A5}$$

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

$$\widehat{T}\left[\mathcal{Y}^{\ell_1\ell_2}_{LM}\Psi(r_1,r_2,r_{12})\right] = -\left[F_0+F_1+F_2+F_3+F_4\right], \tag{A6}$$

where

$$\begin{aligned}
F_0 = \mathcal{Y}^{\ell_1\ell_2}_{LM}&\left\{\frac{1}{2\mu_{13}}\left[\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1}\right] + \frac{1}{\mu_3}\frac{r_1^2+r_2^2-r_{12}^2}{2r_1r_2}\frac{\partial^2}{\partial r_1\partial r_2} + \frac{1}{2\mu_{23}}\left[\frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2}\right]\right.\\
&\left. + \frac{1}{\mu_1}\frac{r_1^2+r_{12}^2-r_2^2}{2r_1r_{12}}\frac{\partial^2}{\partial r_1\partial r_{12}} + \frac{1}{\mu_2}\frac{r_2^2+r_{12}^2-r_1^2}{2r_2r_{12}}\frac{\partial^2}{\partial r_2\partial r_{12}} + \frac{1}{2\mu_{12}}\left[\frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}\right]\right\}\Psi(r_1,r_2,r_{12});
\end{aligned} \tag{A7}$$

and

$$\begin{aligned}
F_1 &= \mathcal{Y}^{\ell_1\ell_2}_{LM}\left\{\frac{\ell_1\partial_1}{\mu_{13}} + \frac{\ell_2\partial_2}{\mu_{23}} + \left(\frac{\ell_1}{\mu_1} + \frac{\ell_2}{\mu_2}\right)\partial_{12}\right\}\Psi(r_1,r_2,r_{12});\\
F_2 &= A\,(\ell_1,\ell_2)\,\mathcal{Y}^{\ell_1-1,\ell_2+1}_{LM}\left\{\frac{\partial_2}{\mu_3} - \frac{\partial_{12}}{\mu_1}\right\}\Psi(r_1,r_2,r_{12});\\
F_3 &= A\,(\ell_2,\ell_1)\,\mathcal{Y}^{\ell_1+1,\ell_2-1}_{LM}\left\{\frac{\partial_1}{\mu_3} - \frac{\partial_{12}}{\mu_2}\right\}\Psi(r_1,r_2,r_{12});\\
F_4 &= \mathcal{Y}^{\ell_1-1,\ell_2-1}_{LM}\left\{\frac{1}{\mu_3}\left[B\,(\ell_1,\ell_2)\,r_2^2\partial_2 + B\,(\ell_2,\ell_1)\,r_1^2\partial_1 + C\,(\ell_1,\ell_2)\right]\right.\\
&\quad\left. - \frac{1}{\mu_1}B\,(\ell_1,\ell_2)\,r_2^2\partial_{12} - \frac{1}{\mu_2}B\,(\ell_2,\ell_1)\,r_1^2\partial_{12}\right\}\Psi(r_1,r_2,r_{12}),
\end{aligned} \tag{A8}$$

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 Δ and ∇ on $\mathcal{Y}^{\ell_1\ell_2}_{LM}(\mathbf{r}_1,\mathbf{r}_2)$ 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

$$I^{L'M'\ell_1'\ell_2'}_{LM\ell_1\ell_2}(\theta_{12}) = \int d\Omega \mathrm{Y}^{\ell_1'\ell_2'}_{L'M'}(\mathbf{r}_1,\mathbf{r}_2)\mathrm{Y}^{\ell_1\ell_2}_{LM}(\mathbf{r}_1,\mathbf{r}_2), \qquad \text{(B1)}$$

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

$$\{Y_l(\hat{\mathbf{r}}_1) \otimes Y_l(\hat{\mathbf{r}}_2)\}_{00} = \frac{(-1)^l(2l+1)^{1/2}}{4\pi} P_l(\cos\theta_{12}). \qquad \text{(B2)}$$

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

$$\begin{aligned} Y_{2m} &= \sqrt{4\pi}\; Y^{20}_{2m}, \\ Y_{2m}(\hat{\mathbf{r}}_{12}) &= \sqrt{4\pi}\left(\frac{r_1^2}{r_{12}^2}Y^{20}_{2m} + \frac{r_2^2}{r_{12}^2}Y^{02}_{2m} - \sqrt{\frac{10}{3}}\,\frac{r_1r_2}{r_{12}^2}Y^{11}_{2m}\right), \end{aligned} \qquad \text{(B3)}$$

and for the matrix elements

$$\left\langle L'l_1'l_2'\|Y_2^{20}\|Ll_1l_2\right\rangle = (-1)^{l_1+l_2+L}\,\frac{\sqrt{5}}{4\pi}\,\Pi_{LL'l_1l_2}\,C^{l_1'0}_{20;l_10}\begin{Bmatrix} l_1 & l_2 & L \\ L' & 2 & l_1' \end{Bmatrix}; \qquad \text{(B4)}$$

$$\left\langle L'l_1'l_2'\|Y_2^{11}\|Ll_1l_2\right\rangle = \frac{3\sqrt{5}}{4\pi}\,\Pi_{LL'l_1}C^{l_1'0}_{10;l_10}C^{l_2'0}_{10;l_20}\begin{Bmatrix} l_1 & l_2 & L \\ 1 & 1 & 2 \\ l_1' & l_2' & L' \end{Bmatrix}, \qquad \text{(B5)}$$

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

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

We used the following relations:

$$\begin{Bmatrix} l_1' & l_1'' & l \\ l_2' & l_2'' & l \\ L & L & 0 \end{Bmatrix} = \frac{(-1)^{l_1''+l_2'+l+L}}{\sqrt{(2L+1)(2l+1)}}\begin{Bmatrix} l_1' & l_1'' & l \\ l_2'' & l_2' & L \end{Bmatrix}, \qquad C^{00}_{L-MLM} = \frac{(-1)^{L+M}}{\sqrt{2L+1}},$$

$$C^{l0}_{l_1'0l_1''0} = (-1)^{l_1'-l_1''}\sqrt{2l+1}\begin{pmatrix} l_1' & l_1'' & l \\ 0 & 0 & 0 \end{pmatrix}, \qquad C^{l0}_{l_2'0l_2''0} = (-1)^{l_2'-l_2''}\sqrt{2l+1}\begin{pmatrix} l_2' & l_2'' & l \\ 0 & 0 & 0 \end{pmatrix}. \qquad \text{(B6)}$$

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

$$\left\{Y_{l_1'}(\hat{\mathbf{r}}_1) \otimes Y_{l_2'}(\hat{\mathbf{r}}_2)\right\}_{L'M'}\left\{Y_{l_1''}(\hat{\mathbf{r}}_1) \otimes Y_{l_2''}(\hat{\mathbf{r}}_2)\right\}_{L''M''} = \sum_{LM} C^{LM}_{L'M'L''M''}\sum_{l_1l_2} B^{l_1l_2L}_{l_1'l_2'L'l_1''l_2''L''}\left\{Y_{l_1}(\hat{\mathbf{r}}_1) \otimes Y_{l_2}(\hat{\mathbf{r}}_2)\right\}_{LM}, \qquad \text{(B7)}$$

where

$$B^{l_1l_2L}_{l_1'l_2'L'l_1''l_2''L''} = \sqrt{\frac{(2l_1'+1)(2l_2'+1)(2l_1''+1)(2l_2''+1)(2L'+1)(2L''+1)}{(4\pi)^2}}C^{l_10}_{l_1'0l_1''0}C^{l_20}_{l_2'0l_2''0}\begin{Bmatrix} l_1' & l_1'' & l_1 \\ l_2' & l_2'' & l_2 \\ L' & L'' & L \end{Bmatrix}. \qquad \text{(B8)}$$

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

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