

Exact non-Born-Oppenheimer wave functions for three-particle Hookean systems with arbitrary masses

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A Hookean model of a three-body problem for particles with arbitrary masses and charges where two of them interact with each other through a Coulomb potential and with the third through a harmonic potential is presented. It is shown that a condition relating the masses to the harmonic coupling constants must be satisfied in order to render this problem separable. A general exact analytic solution written in terms of the relative interparticle coordinates is given as well as general expressions for the total and binding energies of this three-body system. We apply these results to examine electronic, muonic, antiprotonic, and pionic families of non-Born-Oppenheimer Hookean systems. The first contains the atoms or atomic ions: $\text{Ps}^-(e^+e^-e^-)$, $\text{H}^-(p^+e^-e^-)$, $\text{D}^-(d^+e^-e^-)$, $\text{T}^-(t^+e^-e^-)$, ${}^4\text{He}(he^{+2}e^-e^-)$, and the following molecular ions: $\text{Ps}_2^+(e^-e^+e^+)$, $\text{H}_2^+(e^-p^+p^+)$, $\text{HD}^+(e^-d^+p^+)$, $\text{HT}^+(e^-t^+p^+)$, $\text{DT}^+(e^-d^+t^+)$, $\text{D}_2^+(e^-d^+d^+)$, $\text{T}_2^+(e^-t^+t^+)$. The muonic and antiprotonic families are similar to the electronic ones except that the species are formed replacing e^- by μ^- or p^- . The pionic family comprises exotic atoms containing at least one pion. We also apply these results to two-electron three-dimensional spherical quantum dots and for these systems we examine the effect of electronic correlation, particularly on the singlet-triplet transitions and on the collective motion of the electrons and center of mass leading to “floppy” dynamics.

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I. INTRODUCTION

The three-body problem, both in its classical and quantum mechanical versions, has attracted—and continues to attract—a great deal of attention. The reason has to do with the fact that due to a number of inherent difficulties this problem cannot be considered as fully solved in either of these domains. In classical mechanics, Poincaré’s studies of the three-body problem pointed out the existence of nonintegrable Newtonian dynamical systems and opened the way to the understanding of chaotic phenomena. This led, in turn, to formulations in terms of nonlinear differential equations to which novel solutions have been recently found for specific cases [1–5].

The three-body problem in atomic physics appeared when an attempt was made to extend the semiclassical notions entering in the construction of the Bohr atom in order to explain the spectrum of He. Although almost a century has gone by, the vitality of this problem is attested to by the fact that still now solutions are being presented for particular restricted cases of the Coulomb three-body problem [6–10] or for models based on Gaussian potentials [11] or on inverse-square ones [12].

In quantum mechanics, the insurmountable difficulty encountered in the treatment of a three body problem with Coulombic potentials is the nonseparability of the Schrödinger equation [13]. For this reason, much effort has been devoted to formulating this problem in terms of more tractable two-body systems [14] where Jacobian coordinates are used in order to eliminate from the outset the motion of the center of mass. Then, generally, the remaining six degrees of freedom are expressed in terms of hyperspherical coordinates [15–18]. In addition, Faddeev’s equations, which were originally designed to treat the quantum three-body scattering problem, have also been employed to describe bound states [19–23]. However, the complexities of a quantum mechanical three-body system become apparent when the two-body subsystems are weakly bound or even unbound (Borromean). In those cases the weakly bound states in low angular momentum are very extended and give rise to what has been called “halos.” Also, the Efimov effect, associated with the emergence of weakly bound states in the three-body system when the two-body subsystems show vanishing binding energy (and the scattering wavelength greatly exceeds the force range), appears as a universal long range property of the potential [24–26].

Very extensive literature has accumulated on the applications of the three-body approach in the case of the ${}^4\text{He}$ trimer (for some recent references, see [27,28]). Similarly, these

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methods have also been used to treat some atomic and muonic three-body systems [21,29–33]. Different kinds of model potentials have also been introduced with the aim of simplifying the three-body problem. In this respect, it is interesting to note that the three-body problem with δ interactions cannot be solved for general masses [34]. The problem of establishing sufficient conditions for the existence of a physically allowed solution for three-particles interacting through an inverse-square potential, has been investigated by Pupyshev [35]. The effect of adding an inverse-square term to form a Fues-Kratzer-type potential has also been recently investigated [36]. An exact solution to the quantum version of the rigid three-body problem has been obtained by Ma [23]. The harmonic potential has also attracted a great deal of attention in view of the similarities it presents with the actual potential that confines electrons in quantum dots. Another gratifying feature of this potential is that, in the case of two harmonically confined electrons interacting through a Coulombic potential, it is possible to find analytic solutions for particular values of the coupling parameter [37–45]. The harmonic potential has also been used to model and to obtain analytic solutions for the non-Born-Oppenheimer H_2^+ ion [46] as well as to examine in an approximate fashion the behavior of a confined three-electron system [47].

In the present work, we deal with the Hookean model of the quantum three-body system with masses m_1 , m_2 , and m_3 , where particles two and three (with charges Z_2 and Z_3) interact with each other through a Coulomb potential, and where particles one and two and one and three interact through harmonic potentials with coupling constants K_{12} and K_{13} , respectively. In Sec. II, we show that the ratio of harmonic coupling constants K_{13}/K_{12} must be proportional to the mass ratio m_3/m_2 in order to decouple the Schrödinger equation into three equations which describe: the motion of the whole system in terms of the displacement of a collective coordinate, the relative motion of the interacting particles two and three, and the motion of a quasiparticle (a three-dimensional harmonic oscillator), respectively. In Sec. III, we present an explicit wave function for this general three-body problem written in terms of the interparticle coordinates and give a general formula both for the total and binding energies of this three-body system. In Sec. IV the present non-Born-Oppenheimer Hookean model is applied to describe the behavior of electronic, muonic, antiprotonic, and pionic families of three-body systems. In Sec. V, we also apply this model to discuss the effect of electronic correlation both on the spectra and collective motion of three-dimensional quantum dots. Finally, in Sec. VI we advance some conclusions.

II. THE THREE-BODY PROBLEM WITH COULOMB AND HOOKEAN INTERACTION

A. The Hamiltonian

Consider the following three-body problem for a system of three particles defined in terms of the vectors \mathbf{r}_1 , \mathbf{r}_2 , \mathbf{r}_3 with masses m_1 , m_2 , and m_3 , possessing charges Z_1 , Z_2 , and Z_3 and interacting through the potentials

$$V_{12}(\mathbf{r}_1, \mathbf{r}_2) = K_{12} \frac{e^2}{a_o^3 4\pi\epsilon_0} (\mathbf{r}_1 - \mathbf{r}_2)^2, \quad (1)$$

$$V_{13}(\mathbf{r}_1, \mathbf{r}_3) = K_{13} \frac{e^2}{a_o^3 4\pi\epsilon_0} (\mathbf{r}_1 - \mathbf{r}_3)^2, \quad (2)$$

$$V_{23}(\mathbf{r}_2, \mathbf{r}_3) = \frac{Z_2 Z_3 e^2}{4\pi\epsilon_0 |\mathbf{r}_2 - \mathbf{r}_3|}, \quad (3)$$

where $a_o = \hbar^2 \epsilon_0 / \pi m_e e^2$ is the Bohr radius. The Hamiltonian for this system is

$$\begin{aligned} \hat{H} = & -\frac{\hbar^2}{8\pi^2 m_1} \nabla_{\mathbf{r}_1}^2 - \frac{\hbar^2}{8\pi^2 m_2} \nabla_{\mathbf{r}_2}^2 - \frac{\hbar^2}{8\pi^2 m_3} \nabla_{\mathbf{r}_3}^2 \\ & + K_{12} \frac{e^2}{a_o^3 4\pi\epsilon_0} (\mathbf{r}_1 - \mathbf{r}_2)^2 + K_{13} \frac{e^2}{a_o^3 4\pi\epsilon_0} (\mathbf{r}_1 - \mathbf{r}_3)^2 \\ & + \frac{Z_2 Z_3 e^2}{4\pi\epsilon_0 |\mathbf{r}_2 - \mathbf{r}_3|} \end{aligned} \quad (4)$$

and the (spinless) Schrödinger equation is:

$$\hat{H}\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \mathcal{E}\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3). \quad (5)$$

Let us introduce the relative and center-of-mass coordinates for particles two and three:

$$\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_3, \quad (6)$$

$$\mathbf{s} = \frac{m_2 \mathbf{r}_2 + m_3 \mathbf{r}_3}{m_2 + m_3}. \quad (7)$$

Calling $M_{23} = m_2 + m_3$, the inverse transformations are

$$\mathbf{r}_2 = \mathbf{s} + \frac{m_3}{M_{23}} \mathbf{r}, \quad (8)$$

$$\mathbf{r}_3 = \mathbf{s} - \frac{m_2}{M_{23}} \mathbf{r}. \quad (9)$$

Using these equations in the evaluation of $(\mathbf{r}_1 - \mathbf{r}_2)^2$ and $(\mathbf{r}_1 - \mathbf{r}_3)^2$ and transforming the Laplacians into the coordinate system defined by \mathbf{r}_1 , \mathbf{r} , and \mathbf{s} , we can rewrite the Hamiltonian operator given in Eq. (4) as follows:

$$\begin{aligned} \hat{H} = & -\frac{\hbar^2}{8\pi^2 \mu_{23}} \nabla_{\mathbf{r}}^2 - \frac{\hbar^2}{8\pi^2 M_{23}} \nabla_{\mathbf{s}}^2 - \frac{\hbar^2}{8\pi^2 m_1} \nabla_{\mathbf{r}_1}^2 \\ & + \frac{e^2}{a_o^3 4\pi\epsilon_0} \left\{ (K_{12} + K_{13})(\mathbf{r}_1 - \mathbf{s})^2 + 2 \left(K_{13} \frac{m_2}{M_{23}} - K_{12} \frac{m_3}{M_{23}} \right) \right. \\ & \left. \times (\mathbf{r}_1 - \mathbf{s}) \cdot \mathbf{r} + \left[K_{13} \left(\frac{m_2}{M_{23}} \right)^2 + K_{12} \left(\frac{m_3}{M_{23}} \right)^2 \right] r^2 \right\} \\ & + \frac{Z_2 Z_3 e^2}{4\pi\epsilon_0 r}, \end{aligned} \quad (10)$$

where $\mu_{23} = m_2 m_3 / M_{23}$. Introducing this Hamiltonian into Eq. (5), measuring the distances in bohrs, the energy in hartrees, and the mass in atomic units ($m_e = 1$), we obtain

$$\left[-\frac{1}{2} \frac{1}{\mu_{23}} \nabla_{\mathbf{r}}^2 - \frac{1}{2} \frac{1}{M_{23}} \nabla_{\mathbf{s}}^2 - \frac{1}{2} \frac{1}{m_1} \nabla_{\mathbf{r}_1}^2 + (K_{12} + K_{13})(\mathbf{r}_1 - \mathbf{s})^2 \right. \\ \left. + 2 \left(K_{13} \frac{m_2}{M_{23}} - K_{12} \frac{m_3}{M_{23}} \right) (\mathbf{r}_1 - \mathbf{s}) \cdot \mathbf{r} + \left[K_{13} \left(\frac{m_2}{M_{23}} \right)^2 \right. \right. \\ \left. \left. + K_{12} \left(\frac{m_3}{M_{23}} \right)^2 \right] r^2 + \frac{Z_2 Z_3}{r} \right] \Psi = \mathcal{E} \Psi. \quad (11)$$

B. Separability condition for the Hamiltonian

Equation (11) shows that in spite of the above coordinate transformations, there remain couplings among the new coordinates. The fourth term in the right-hand side (rhs) gives coupling between the coordinates \mathbf{r}_1 and \mathbf{s} and the fifth, between $\mathbf{r}_1 - \mathbf{s}$ and \mathbf{r} . The first coupling can be readily disposed of, as will be shown below. However, in order to eliminate the latter, we must require that its coefficient be zero:

$$\left(K_{13} \frac{m_2}{M_{23}} - K_{12} \frac{m_3}{M_{23}} \right) = 0 \quad (12)$$

which leads to the equation

$$\frac{K_{13}}{K_{12}} = \frac{m_3}{m_2}. \quad (13)$$

One way to fulfill this condition is to require that particles two and three be equal, i.e., that

$$m_2 = m_3 = m \quad \text{and} \quad K_{12} = K_{13} = k. \quad (14)$$

But condition (13) is also satisfied as long as the harmonic coupling constants K_{1i} are proportional (with the same constant of proportionality) to the product of their corresponding masses, i.e., when

$$K_{1i} = a \times m_1 \times m_i \quad \text{for } i = 2, 3. \quad (15)$$

In what follows, to insure the decoupling, we assume that either conditions (14) or (15) hold and obtain:

$$\left[K_{13} \left(\frac{m_2}{M_{23}} \right)^2 + K_{12} \left(\frac{m_3}{M_{23}} \right)^2 \right] r^2 = K_{12} \frac{m_3}{M_{23}} r^2 = K_{13} \frac{m_2}{M_{23}} r^2 \quad (16)$$

and

$$K_{12} + K_{13} = K_{12} \frac{M_{23}}{m_2} = K_{13} \frac{M_{23}}{m_3}. \quad (17)$$

C. Decoupling of Schrödinger's equation

Setting the wave function

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \Psi_{\mathbf{r}}(\mathbf{r}) \Psi_{\mathbf{r}_1, \mathbf{s}}(\mathbf{r}_1, \mathbf{s}) \quad (18)$$

and using Eqs. (16) and (17) we can decouple Eq. (11) into the following:

$$\left[-\frac{1}{2} \frac{1}{\mu_{23}} \nabla_{\mathbf{r}}^2 + K_{13} \frac{m_2}{M_{23}} r^2 + \frac{Z_2 Z_3}{r} \right] \Psi_{\mathbf{r}}(\mathbf{r}) = \mathcal{E}_{\mathbf{r}} \Psi_{\mathbf{r}}(\mathbf{r}) \quad (19)$$

and

$$\left[-\frac{1}{2} \frac{1}{M_{23}} \nabla_{\mathbf{s}}^2 - \frac{1}{2} \frac{1}{m_1} \nabla_{\mathbf{r}_1}^2 + K_{13} \frac{M_{23}}{m_3} (\mathbf{r}_1 - \mathbf{s})^2 \right] \Psi_{\mathbf{r}_1, \mathbf{s}}(\mathbf{r}_1, \mathbf{s}) \\ = \mathcal{E}'_{\mathbf{r}_1, \mathbf{s}} \Psi_{\mathbf{r}_1, \mathbf{s}}(\mathbf{r}_1, \mathbf{s}). \quad (20)$$

Now, expanding $(\mathbf{r}_1 - \mathbf{s})^2$ and multiplying by m_1 we can re-write Eq. (20) in the general form:

$$\left[-\frac{1}{2} \frac{1}{M} \nabla_{\mathbf{s}}^2 - \frac{1}{2} \nabla_{\mathbf{r}_1}^2 + 4\omega^2 (r_1^2 + s^2 - 2\mathbf{r}_1 \cdot \mathbf{s}) \right] \Psi_{\mathbf{r}_1, \mathbf{s}}(\mathbf{r}_1, \mathbf{s}) \\ = \mathcal{E}'_{\mathbf{r}_1, \mathbf{s}} \Psi_{\mathbf{r}_1, \mathbf{s}}(\mathbf{r}_1, \mathbf{s}), \quad (21)$$

where we have defined

$$M = M_{23}/m_1, \quad 4\omega^2 = K_{13} \frac{m_1 M_{23}}{m_3}, \quad \mathcal{E}'_{\mathbf{r}_1, \mathbf{s}} = m_1 \mathcal{E}_{\mathbf{r}_1, \mathbf{s}}. \quad (22)$$

Equation (21) may be put in a more convenient form by introducing the auxiliary variable $\tilde{\mathbf{s}} = \sqrt{M}\mathbf{s}$:

$$\left[-\frac{1}{2} \nabla_{\tilde{\mathbf{s}}}^2 - \frac{1}{2} \nabla_{\mathbf{r}_1}^2 + 4\omega^2 \left(r_1^2 + \frac{\tilde{s}^2}{M} - \frac{2\mathbf{r}_1 \cdot \tilde{\mathbf{s}}}{\sqrt{M}} \right) \right] \Psi_{\mathbf{r}_1, \tilde{\mathbf{s}}}(\mathbf{r}_1, \tilde{\mathbf{s}}) \\ = \mathcal{E}'_{\mathbf{r}_1, \tilde{\mathbf{s}}} \Psi_{\mathbf{r}_1, \tilde{\mathbf{s}}}(\mathbf{r}_1, \tilde{\mathbf{s}}), \quad (23)$$

where $\mathcal{E}'_{\mathbf{r}_1, \tilde{\mathbf{s}}} = \mathcal{E}_{\mathbf{r}_1, \tilde{\mathbf{s}}}$. Observe that this equation can be decoupled through coordinates \mathbf{P} and \mathbf{Q} defined by means of the unitary rotation

$$\begin{pmatrix} \mathbf{P} \\ \mathbf{Q} \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \mathbf{r}_1 \\ \tilde{\mathbf{s}} \end{pmatrix} \quad (24)$$

of angle $\theta = \tan^{-1}(M)$. With this transformation Eq. (21) can be cast as follows:

$$\left[-\frac{1}{2} \nabla_{\mathbf{P}}^2 - \frac{1}{2} \nabla_{\mathbf{Q}}^2 + \frac{4\omega^2(M+1)}{M} Q^2 \right] \Psi_{\mathbf{P}, \mathbf{Q}}(\mathbf{P}, \mathbf{Q}) \\ = \mathcal{E}_{\mathbf{P}, \mathbf{Q}} \Psi_{\mathbf{P}, \mathbf{Q}}(\mathbf{P}, \mathbf{Q}). \quad (25)$$

Taking $\Psi_{\mathbf{P}, \mathbf{Q}}(\mathbf{P}, \mathbf{Q}) = \Psi_{\mathbf{P}}(\mathbf{P}) \Psi_{\mathbf{Q}}(\mathbf{Q})$ we obtain the following decoupled equations:

$$-\frac{1}{2} \nabla_{\mathbf{P}}^2 \Psi_{\mathbf{P}}(\mathbf{P}) = \mathcal{E}_{\mathbf{P}} \Psi_{\mathbf{P}}(\mathbf{P}) \quad (26)$$

and

$$\left[-\frac{1}{2} \nabla_{\mathbf{Q}}^2 + \frac{W_{\mathbf{Q}}^2}{2} Q^2 \right] \Psi_{\mathbf{Q}}(\mathbf{Q}) = \mathcal{E}_{\mathbf{Q}} \Psi_{\mathbf{Q}}(\mathbf{Q}), \quad (27)$$

where we have defined

$$\frac{W_{\mathbf{Q}}^2}{2} = 4\omega^2 \frac{(M+1)}{M} \quad (28)$$

and where, in view of Eq. (22) the energy is

$$\mathcal{E}_{\mathbf{r}_1, \mathbf{s}} = \frac{\mathcal{E}_{\mathbf{P}} + \mathcal{E}_{\mathbf{Q}}}{m_1}. \quad (29)$$

D. Solution to the relative motion equation

Multiplying Eq. (19) by μ_{23} , we obtain the equation:

$$\left[-\frac{1}{2}\nabla_{\mathbf{r}}^2 + \frac{W_r^2}{2}r^2 + \frac{K_r}{2r} \right] \Psi_{\mathbf{r}}(\mathbf{r}) = \mathcal{E}'_r \Psi_{\mathbf{r}}(\mathbf{r}), \quad (30)$$

where, bearing in mind Eq. (22) we have defined

$$\frac{W_r^2}{2} = K_{13}\mu_{23}\frac{m_2}{M_{23}}, \quad K_r = 2Z_2Z_3\mu_{23}, \quad \text{and } \mathcal{E}'_r = \mu_{23}\mathcal{E}_r. \quad (31)$$

The wave function appearing in Eq. (30) can be separated into its radial and angular parts $\Psi_{\mathbf{r}}(\mathbf{r}) = \psi_r(r)Y_{l_r, m_r}(\theta_r, \varphi_r)$ and as a result, setting $\psi_r(r) = \mu_r(r)/r$ we obtain the following equation for the radial part:

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l_r(l_r+1)}{2r^2} + \frac{K_r}{2r} + \frac{W_r^2}{2}r^2 \right] \mu_r(r) = \mathcal{E}'_r \mu_r(r). \quad (32)$$

The general solution to this equation is

$$\mu_{n_r, l_r}(r) = r^{l_r+1} \exp\left(-\frac{W_r(n_r, l_r)}{2}r^2\right) \sum_{i=0}^{n_r} a_i r^i, \quad (33)$$

where we have emphasized the dependence of the coupling constant $W_r(n_r, l_r)$ on the quantum numbers. For any specific pair of quantum numbers n_r, l_r , the coupling constant $W_r(n_r, l_r)$ is determined through the solution of the recursion relations for the expansion coefficients [43].

The corresponding energy is given by

$$\mathcal{E}'_r = W_r(n_r, l_r) \left(n_r + l_r + \frac{3}{2} \right). \quad (34)$$

E. Solution to the equation for the quasiparticle motion

Equation (27) describes the motion of a three-dimensional harmonic oscillator whose wave function can be written as the product of a radial and an angular part, i.e., $\Psi_{\mathbf{Q}}(\mathbf{Q}) = \psi_{\nu_Q}(Q)Y_{\nu_Q, l_Q}(\theta_Q, \varphi_Q)$ where the radial part is given by

$$\begin{aligned} \psi_{\nu_Q, l_Q}(Q) &= N_{\nu_Q, l_Q} Q^{l_Q} \exp[-(W_Q/2)Q^2] \\ &\times F(-\nu_Q, l_Q + 3/2, W_Q Q^2) \end{aligned} \quad (35)$$

and where $F(-\nu_Q, l_Q + 3/2, W_Q Q^2)$ is the confluent hypergeometric function.

Note, in view of Eqs. (22) the coupling parameters are connected and satisfy the explicit relations:

$$W_Q(n_r, l_r) = \frac{\sqrt{M_{123}}\sqrt{m_1}}{\mu_{23}} W_r(n_r, l_r), \quad (36)$$

$$\mathcal{E}'_{0,0} = \frac{3}{2}\sqrt{M_{123}}\mu_{23}\sqrt{m_1}Z_2^2Z_3^2, \quad (37)$$

where $M_{123} = m_1 + m_2 + m_3$. Since we take $\mathcal{E}_p = 0$ (we measure the energy of the system with respect to that of the collective

displacement), bearing in mind Eqs. (29) and (37), we finally obtain:

$$\mathcal{E}_{r_1, s} = \frac{3}{2}\sqrt{\frac{M_{123}}{m_1}}\mu_{23}Z_2^2Z_3^2. \quad (38)$$

III. EXPLICIT REPRESENTATIONS FOR THE TOTAL WAVE FUNCTION AND EXPLICIT FORMS OF THE TOTAL AND BINDING ENERGIES

Another consequence of setting $\mathcal{E}_p = 0$ is that the wave function $\Psi_{\mathbf{P}}(\mathbf{P})$ becomes a constant and can be disregarded (note that this deletion does not arise from taking $\mathbf{P} = 0$ as the origin of the coordinate system). As a consequence, the total three-particle wave function corresponding to the quantum numbers n_r, l_r , and ν_Q, l_Q can be written:

$$\begin{aligned} \Psi_{n_r, l_r, \nu_Q, l_Q}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \\ = \frac{1}{4\pi} \psi_{n_r, l_r}(r) \psi_{\nu_Q, l_Q}(Q) \mathcal{Y}_{l_r, m_r}(\Omega_r) \mathcal{Y}_{l_Q, m_Q}(\Omega_Q). \end{aligned} \quad (39)$$

Actually, the individual spherical harmonics must couple to form a total angular momentum eigenfunction characterized by the global quantum numbers L and M . In fact, similar methods to those discussed by Frolov and Smith [48] (see also Refs. [49,50]) may be used here to generate the global wave function $\Psi_{n_r, \nu_Q, L, M}(\mathbf{r}, \mathbf{Q})$. For simplicity, we only consider here the totally symmetric ground-state case with $L = 0$ and $M = 0$ which corresponds to $l_r = 0$ and $l_Q = 0$ and is described by the wave function:

$$\Psi_{n_r, 0, \nu_Q, 0}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \frac{1}{4\pi} \psi_{n_r, 0}(r) \psi_{\nu_Q, 0}(Q). \quad (40)$$

A. Interparticle coordinate representation

Using Eqs. (6) and (61) we have $r^2 \equiv r_{23}^2$ and

$$Q^2 = \frac{m_2}{M_{123}}r_{12}^2 + \frac{m_3}{M_{123}}r_{13}^2 - \frac{\mu_{23}}{M_{123}}r_{23}^2. \quad (41)$$

Hence, the general form of the total wave functions is:

$$\begin{aligned} \Psi_{n_r, 0, \nu_Q, 0}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) &= \frac{N_{n_r, 0}^r N_{\nu_Q, 0}^Q}{4\pi} \left(\sum_{i=0}^{n_r} a_i r_{23}^i \right) \\ &\times \exp(-\alpha_{12}r_{12}^2 - \alpha_{13}r_{13}^2 - \alpha_{23}r_{23}^2) \\ &\times F(-\nu_Q, 3/2, W_Q Q^2), \end{aligned} \quad (42)$$

where

$$\alpha_{23} = \frac{1}{2} \left(W_r(n_r, 0) - \sqrt{\frac{m_1}{M_{123}}} \mu_{23} \right)^2 Z_2^2 Z_3^2, \quad (43)$$

$$\alpha_{12} = \frac{1}{2} \sqrt{\frac{m_1}{M_{123}}} \mu_{23} m_2 Z_2^2 Z_3^2, \quad (44)$$

$$\alpha_{13} = \frac{1}{2} \sqrt{\frac{m_1}{M_{123}}} \mu_{23} m_3 Z_2^2 Z_3^2, \quad (45)$$

and where the argument of the confluent hypergeometric function is:

$$W_{Q^2} = W_r(n_r, 0) \frac{1}{\mu_{23}} \sqrt{\frac{m_1}{M_{123}}} (m_2 r_{12}^2 + m_3 r_{13}^2 - \mu_{23} r_{23}^2). \quad (46)$$

In the treatment of the Coulombic case, it is customary to express the variational wave function [48,51] in terms of the basis functions $\{\chi_i(r_{12}, r_{13}, r_{23}) = \exp(-\alpha_i r_{23} - \beta_i r_{13} - \gamma_i r_{12})\}$ which explicitly contain the interparticle coordinates. It is observed that the exact Hookean solution given by Eq. (42) has this general form, except for the fact that due to harmonic confinement we have Gaussians instead of exponential functions. Moreover, in the exact Hookean case, the parameters α_{ij} are totally determined by the quantum numbers, the masses, and the charges. Another interesting fact is the appearance in the Hookean system of a correlation function for the particles with the same charge (two and three) whose order is determined by the quantum number n_r . As we show below, the order of this polynomial can be quite large ($n_r = 65$, for example, for H_2^+) when the Hookean wave function is constrained to yield a $\langle r \rangle$ value close to that of the Coulombic system.

B. Electronic and nuclear coordinate representation

In the work of Bishop and Cheung [52] the wave function for a Coulombic three-body system, say H_2^+ , is written in terms of the internuclear distance $R = r_{23}$ and of the vector $\mathbf{r}_e = (r_e, \theta_e, \varphi_e)$ denoting the relative position of the electron with respect to the nuclear geometric center. Hence, $\mathbf{r}_e = \mathbf{r}_1 - \mathbf{s}$, where $\mathbf{s} = (\mathbf{r}_2 + \mathbf{r}_3)/2$. The connection of this representation with the present one can be readily established by noting that the coordinate \mathbf{Q} may be written:

$$\mathbf{Q} = -\sqrt{\frac{M_{23}}{M_{123}}} (\mathbf{r}_1 - \mathbf{s}) = -\sqrt{\frac{M_{23}}{M_{123}}} \mathbf{r}_e. \quad (47)$$

However, in contrast with Bishop and Cheung's definition, in the present case [see Eq. (7)], \mathbf{s} is the nuclear center of mass. But, since for homonuclear diatomic molecules, the nuclear and the geometric center of mass coincide, we see that the exact Hookean wave function in this case can be expressed in terms of the electronic and nuclear coordinates:

$$\Psi_{n_r, 0, \nu_Q, 0}(\mathbf{r}_{23}, \mathbf{Q}) = \frac{1}{\sqrt{4\pi}} \psi_{n_r, 0}(R) \tilde{\Psi}_{\nu_Q, 0}(r_e, \theta_e, \varphi_e). \quad (48)$$

Note, moreover, that the vector \mathbf{r}_e can also be expressed, as it is done in the treatment of Bishop and Cheung [53], in terms of prolate spheroidal coordinates as $\mathbf{r}_e = (\xi, \eta, \varphi)$, where $\xi = (r_{12} + r_{13})/R$ and $\eta = (r_{12} - r_{13})/R$.

C. Total energy and binding energies

The total energy depends on the quantum numbers and can be written:

$$\mathcal{E}_T = \mathcal{E}_r + \mathcal{E}_{r_{1,s}} = \frac{1}{\mu_{23}} W_r(n_r, l_r) \left[\left(n_r + l_r + \frac{3}{2} \right) + \sqrt{\frac{M_{123}}{m_1}} \left(2\nu_Q + l_Q + \frac{3}{2} \right) \right]. \quad (49)$$

Finally, the binding energy $\mathcal{E}_i^B = \mathcal{E}_T - \mathcal{E}_i^{\text{at}}$, defined as the difference between the total energy for the three-body system \mathcal{E}_T and that of an "atom," $\mathcal{E}_i^{\text{at}}$ consisting of particles one and i ($i=2,3$), is given by

$$\mathcal{E}_i^B = \frac{1}{\mu_{23}} W_r(n_r, l_r) \left[\left(n_r + l_r + \frac{3}{2} \right) + \sqrt{\frac{M_{123}}{m_1}} \left(2\nu_Q + l_Q + \frac{3}{2} \right) - \sqrt{\frac{\mu_{23}}{\mu_{1i}}} \sqrt{\frac{M_{23}}{m_j}} \left(2\tilde{n}_r + \tilde{l}_r + \frac{3}{2} \right) \right] \quad (50)$$

for $i \neq j$, where \tilde{n}_r and \tilde{l}_r are the quantum numbers for the "atom." We assume, moreover, that the same molecular harmonic coupling constant also holds in the case of the "atom."

IV. APPLICATION TO THREE-BODY SYSTEMS

There exists a large number of Coulomb three-body systems that over the years have attracted much attention. These systems have been thoroughly studied by means of approximate methods. The latter, in view of the extreme precision required for a proper description of these systems, have undergone considerable refinements.

Among the most studied three-particle systems, we may distinguish the following families: electronic, muonic, antiprotonic, and pionic. The family of electronic three-particle systems is formed by the following atoms (or atomic ions): $\text{Ps}^-(e^+e^-e^-)$, $\text{H}^-(p^+e^-e^-)$, $\text{D}^-(d^+e^-e^-)$, $\text{T}^-(t^+e^-e^-)$, ${}^4\text{He}(he^{+2}e^-e^-)$ and its finite-nuclei isoelectronic series, and the following molecular ions: $\text{Ps}_2^+(e^-e^+e^+)$, $\text{H}_2^+(e^-p^+p^+)$, $\text{HD}^+(e^-d^+p^+)$, $\text{HT}^+(e^-t^+p^+)$, $\text{DT}^+(e^-d^+t^+)$, $\text{D}_2^+(e^-d^+d^+)$, $\text{T}_2^+(e^-t^+t^+)$. The family of muonic systems is similar to that of electronic ones except that the species are formed replacing e^- by the negative muon μ^- . Similarly, the family of antiprotonic systems is generated by replacing e^- by the antiproton p^- . Finally, under the denomination of pionic systems we consider the family of exotic atoms and molecules resulting from the combinations of at least one positive or negative pion with muons (positive and negative), electrons, positrons, protons, and antiprotons.

Results of the Hookean model calculations for atomic and molecular electronic systems are presented in Tables I and II, respectively. Similarly, those for muonic, antiprotonic and pionic systems are listed in Tables III–V, respectively. The data for electronic systems listed in Tables I and II is given in hartrees for the energy and in bohrs for the length. Unless explicitly stated, the data in the remaining tables is presented in muonic units of energy (hartree/ $m_\mu = \mu.u.$) and muonic units of distance (bohr $\times m_\mu = \mu.u.$). In these tables, \mathcal{E}_r denotes the internal energy for the Coulombic interaction of particles two and three in the harmonic potential field produced by particle one. The value of \mathcal{E}_r has been decomposed into its kinetic (\mathcal{E}_r^K), repulsion (\mathcal{E}_r^R), and confinement (\mathcal{E}_r^C)

TABLE I. Hookean model results for three-body electronic atomic systems. The n_r values denote the degree of correlation, Eq. (33). Data in electronic atomic units.

Atom	Ps ⁻ $e^+e^-e^-$	H ⁻ $p^+e^-e^-$	D ⁻ $d^+e^-e^-$	T ⁻ $t^+e^-e^-$	⁴ He $he^{+2}e^-e^-$
n_r	1	1	1	1	1
W_r	2.500000×10^{-1}	2.500000×10^{-1}	2.500000×10^{-1}	2.500000×10^{-1}	2.500000×10^{-1}
\mathcal{E}_r^K	2.894176×10^{-1}	2.894176×10^{-1}	2.894176×10^{-1}	2.894176×10^{-1}	2.894176×10^{-1}
\mathcal{E}_r^R	4.474432×10^{-1}	4.474432×10^{-1}	4.474432×10^{-1}	4.474432×10^{-1}	4.474432×10^{-1}
\mathcal{E}_r^C	5.131392×10^{-1}	5.131392×10^{-1}	5.131392×10^{-1}	5.131392×10^{-1}	5.131392×10^{-1}
\mathcal{E}_r	1.250000	1.250000	1.250000	1.250000	1.250000
$\mathcal{E}_{r_{1,s}}$	1.299038	7.504084×10^{-1}	7.502043×10^{-1}	7.501364×10^{-1}	7.501020×10^{-1}
\mathcal{E}_T	2.549038	2.000408	2.000204	2.000136	2.000102
\mathcal{E}_3^B	1.488378	1.250204	1.250102	1.250068	1.250051
\mathcal{E}_2^B	1.488378	1.250204	1.250102	1.250068	1.250051
$\langle r \rangle$	2.684659	2.684659	2.684659	2.684659	2.684659
$\langle Q \rangle$	1.212522	3.723038×10^{-2}	2.633597×10^{-2}	2.152141×10^{-2}	1.861258×10^{-2}
n_r	3	2			
W_r	1.826863×10^{-2}	5.000000×10^{-2}			
\mathcal{E}_r^K	1.764072×10^{-2}	5.102834×10^{-2}			
\mathcal{E}_r^R	8.609083×10^{-2}	1.652955×10^{-1}			
\mathcal{E}_r^C	6.068614×10^{-2}	1.336761×10^{-1}			
\mathcal{E}_r	1.644177×10^{-1}	3.500000×10^{-1}			
$\mathcal{E}_{r_{1,s}}$	9.492660×10^{-2}	1.500817×10^{-1}			
\mathcal{E}_T	2.593443×10^{-1}	5.000817×10^{-1}			
\mathcal{E}_3^B	1.818371×10^{-1}	3.500408×10^{-1}			
\mathcal{E}_2^B	1.818371×10^{-1}	3.500408×10^{-1}			
$\langle r \rangle$	$1.292418 \times 10^{+1}$	6.942413			
$\langle Q \rangle$	4.485457	8.324966×10^{-2}			
$\langle r \rangle_{Coul}$	8.548580[54]	4.415693[55]			1.422248[55]

energy components. The reported energy $\mathcal{E}_{r_{1,s}} = \mathcal{E}_Q/m_1$ is essentially the energy of a “particle” whose wave function is described by the collective coordinate \mathbf{Q} coupling the motion of particle one with the center of mass of particles two and three. It follows, in view of Eq. (47), that this is the energy resulting from the vibration of the collective coordinate \mathbf{Q} . The energy shown in the tables corresponds to the $\nu=0$ and $l_Q=0$ level of the three-dimensional harmonic oscillator. Note that in this case there is no need to decompose this energy as the kinetic and potential energy components are coupled by the virial theorem. The total energy \mathcal{E}_T corresponds to the sum of \mathcal{E}_r and $\mathcal{E}_{r_{1,s}}$ and is given in general form by Eq. (49). Binding energies with respect to the dissociation of the three-particle system into an atom containing particles one and i ($i=2,3$) are calculated by means of Eq. (50).

The results presented in the upper part of these tables correspond to $n_r=1$ and, hence, they refer to the simplest correlated wave function. In addition to the values of $\langle r \rangle$ computed for $n_r=1$ we have listed for comparison purposes at the bottom of these tables the reported average values, $\langle r \rangle_{Coul}$, (whenever available in the literature) for full Coulombic interaction.

In order to establish a closer correspondence between the model Hookean calculations presented here and real Cou-

lomb systems, we have searched for ground state solutions of the Hookean model [Eq. (33)] corresponding to different n_r values such that the average values of the interparticle distances $\langle r \rangle$ are larger, but lie as close as possible to the $\langle r \rangle_{Coul}$ ones. These results are reported in the lower part of the tables. Thus, for example, in the lower part of Table II we present for H_2^+ and HD^+ results obtained for $n_r=65$ and $n_r=75$, respectively, which yield $\langle r \rangle=2.099$ bohrs ($\langle r \rangle_{Coul}=2.063$ bohrs) for H_2^+ and $\langle r \rangle=2.089$ bohrs ($\langle r \rangle_{Coul}=2.055$ bohrs) for HD^+ . It is clear that the wave functions for $n_r > 1$ reported in the present calculations correspond in almost all cases to very highly correlated interparticle wave functions of the type described by Eq. (33).

V. APPLICATION TO QUANTUM-DOT SYSTEMS

In the present section we use the Hookean three-body model to examine electron correlation in a two-electron spherical quantum dot and, in particular, to assess the influence of finite and infinite masses of either the quantum dot or impurities on the collective dynamics of this system. Three-dimensional spherical quantum dots have been realized experimentally only recently through the use of colloidal semiconductor nanocrystals [59,60]. (In contrast, two-

TABLE II. Hookean model results for three-body electronic molecular ions. Data in electronic atomic units.

Molecule	H_2^+ $e^-p^+p^+$	HD^+ $e^-d^+p^+$	HT^+ $e^-t^+p^+$	D_2^+ $e^-d^+d^+$	DT^+ $e^-t^+d^+$	T_2^+ $e^-t^+t^+$
n_r	1	1	1	1	1	1
W_r	$8.428642 \times 10^{+5}$	$1.497929 \times 10^{+6}$	$1.894456 \times 10^{+6}$	$3.368111 \times 10^{+6}$	$4.843873 \times 10^{+6}$	$7.554037 \times 10^{+6}$
\mathcal{E}_r^K	$5.314149 \times 10^{+2}$	$7.084360 \times 10^{+2}$	$7.967043 \times 10^{+2}$	$1.062302 \times 10^{+3}$	$1.273947 \times 10^{+3}$	$1.590906 \times 10^{+3}$
\mathcal{E}_r^R	$8.215740 \times 10^{+2}$	$1.095251 \times 10^{+3}$	$1.231715 \times 10^{+3}$	$1.642333 \times 10^{+3}$	$1.969538 \times 10^{+3}$	$2.459560 \times 10^{+3}$
\mathcal{E}_r^C	$9.422019 \times 10^{+2}$	$1.256061 \times 10^{+3}$	$1.412562 \times 10^{+3}$	$1.883469 \times 10^{+3}$	$2.258716 \times 10^{+3}$	$2.820686 \times 10^{+3}$
\mathcal{E}_r	$2.295191 \times 10^{+3}$	$3.059748 \times 10^{+3}$	$3.440981 \times 10^{+3}$	$4.588104 \times 10^{+3}$	$5.502200 \times 10^{+3}$	$6.871152 \times 10^{+3}$
$\mathcal{E}_{r_{1,s}}$	$8.346388 \times 10^{+4}$	$1.362447 \times 10^{+5}$	$1.768097 \times 10^{+5}$	$2.358798 \times 10^{+5}$	$3.161073 \times 10^{+5}$	$4.322901 \times 10^{+5}$
\mathcal{E}_T	$8.575907 \times 10^{+4}$	$1.393044 \times 10^{+5}$	$1.802507 \times 10^{+5}$	$2.404679 \times 10^{+5}$	$3.216095 \times 10^{+5}$	$4.391613 \times 10^{+5}$
\mathcal{E}_3^B	$2.673316 \times 10^{+4}$	$2.806526 \times 10^{+4}$	$2.716566 \times 10^{+4}$	$7.366433 \times 10^{+4}$	$7.682331 \times 10^{+4}$	$1.334721 \times 10^{+5}$
\mathcal{E}_2^B	$2.673316 \times 10^{+4}$	$6.061623 \times 10^{+4}$	$9.175828 \times 10^{+4}$	$7.366433 \times 10^{+4}$	$1.215734 \times 10^{+5}$	$1.334721 \times 10^{+5}$
$\langle r \rangle$	1.462111×10^{-3}	1.096765×10^{-3}	9.752521×10^{-4}	7.314185×10^{-4}	6.099059×10^{-4}	4.883932×10^{-4}
$\langle Q \rangle$	4.783562×10^{-3}	3.744044×10^{-3}	3.286606×10^{-3}	2.845479×10^{-3}	2.458009×10^{-3}	2.101905×10^{-3}
n_r	65	75				
W_r	$1.006212 \times 10^{+1}$	$1.168541 \times 10^{+1}$				
\mathcal{E}_r^K	4.770370×10^{-3}	4.151491×10^{-3}				
\mathcal{E}_r^R	4.795329×10^{-1}	4.813823×10^{-1}				
\mathcal{E}_r^C	2.445372×10^{-1}	2.448665×10^{-1}				
\mathcal{E}_r	7.288404×10^{-1}	7.303982×10^{-1}				
$\mathcal{E}_{r_{1,s}}$	9.963927×10^{-1}	1.062850				
\mathcal{E}_T	1.725233	1.793249				
\mathcal{E}_3^B	1.020581	9.254673×10^{-1}				
\mathcal{E}_2^B	1.020581	1.179399				
$\langle r \rangle$	2.099100	2.089231				
$\langle Q \rangle$	1.384476	1.340493				
$\langle r \rangle_{Coul}$	2.063913[55]	2.055[56]				

dimensional (2D) quantum dots were produced almost two decades ago [61,62].)

Recently, the excitation spectrum of two-electron (2D) quantum dots has been investigated by tunneling spectroscopy [63] and the theoretical prediction of singlet-triplet transitions with increasing magnetic field has been experimentally corroborated. This, in turn, reinforces the suggestion that these states may be used as those of a qubit, or that these two-electron dots may be employed to implement logical gates in quantum computing.

In two-electron quantum dots as well as in those containing $N > 2$ electrons the incorporation of electron correlation effects has been shown to be essential for an adequate interpretation of their experimental spectra and transport properties [64–67]. However, in quantum dots, as opposed to real atoms, the effect of electron correlation may be varied at will through manipulation of the dimension and shape of the nanocrystal as well as of the strength, boundaries, and symmetries of the confining fields [68,69]. This fact makes the quantum dot many-body problem much more complex than the usual atomic one.

Due to the intrinsic nonseparability of Coulomb electron-electron interaction in N -electron quantum dots, the correlation problem cannot be treated analytically. In view of this

fact, approximate descriptions of quantum dots have been advanced where the electron-electron interaction is treated, for example, via a constant interaction model [70] or where, keeping the interaction unchanged, approximations based on infinite-barrier quantum-well boxes (parallelepipeds [71] and spheres [72,73]) are used. Also, for the actual interactions and boundaries, several usual quantum chemistry methods have been used. Among these, we have diagonalizations of large configuration interaction representations of the Hamiltonian matrix (these are usually referred as “exact” diagonalizations) [74–80], Hartree-Fock calculations [78,81–85], (including coupled-cluster-type ones [86]), density functional theory applications [87–90], and, finally, quantum Monte Carlo calculations [91]. Let us remark, however, that even for two-electron quantum dots it is observed that in order to incorporate correlation properly, one must go beyond perturbative schemes based on the independent-particle picture or spin-density functional theory [63].

Customarily, two interacting electrons in a two- or three-dimensional quantum dot model are led in terms of a harmonic trapping potential [43,69,92–95]. (For generalizations, see Refs. [47,96].) The advantage of such a two-particle model is that it has analytical closed-form solutions for certain values of the harmonic confining parameter (or equiva-

TABLE III. Hookean model results for three-body muonic systems (atoms and molecules). Data in muonic units.

Atom	$e^+\mu^-\mu^-$	$p^+\mu^-\mu^-$	$d^+\mu^-\mu^-$	$t^+\mu^-\mu^-$	$he^{+2}\mu^-\mu^-$	Molecule	$\mu^-p^+p^+$	$\mu^-d^+p^+$	$\mu^-t^+p^+$	$\mu^-d^+d^+$	$\mu^-t^+d^+$	$\mu^-t^+t^+$
n_r	1	1	1	1	1	n_r	1	1	1	1	1	1
W_r	$5.169207 \times 10^{+1}$	$5.169207 \times 10^{+1}$	$5.169207 \times 10^{+1}$	$5.169207 \times 10^{+1}$	$5.169207 \times 10^{+1}$	W_r	$4.076371 \times 10^{+3}$	$7.244484 \times 10^{+3}$	$9.162218 \times 10^{+3}$	$1.628931 \times 10^{+4}$	$2.342658 \times 10^{+4}$	$3.653383 \times 10^{+4}$
\mathcal{E}_r^K	2.894176×10^{-1}	2.894176×10^{-1}	2.894176×10^{-1}	2.894176×10^{-1}	2.894176×10^{-1}	\mathcal{E}_r^K	2.570099	3.426232	3.853127	5.137647	6.161230	7.694149
\mathcal{E}_r^R	4.474432×10^{-1}	4.474432×10^{-1}	4.474432×10^{-1}	4.474432×10^{-1}	4.474432×10^{-1}	\mathcal{E}_r^R	3.973405	5.296997	5.956982	7.942866	9.525338	$1.189525 \times 10^{+1}$
\mathcal{E}_r^C	5.131392×10^{-1}	5.131392×10^{-1}	5.131392×10^{-1}	5.131392×10^{-1}	5.131392×10^{-1}	\mathcal{E}_r^C	4.556802	6.074730	6.831618	9.109080	$1.092390 \times 10^{+1}$	$1.364177 \times 10^{+1}$
\mathcal{E}_r	1.250000	1.250000	1.250000	1.250000	1.250000	\mathcal{E}_r	$1.110031 \times 10^{+1}$	$1.479796 \times 10^{+1}$	$1.664173 \times 10^{+1}$	$2.218959 \times 10^{+1}$	$2.661047 \times 10^{+1}$	$3.323117 \times 10^{+1}$
$\mathcal{E}_{r_{1,s}}$	$1.527013 \times 10^{+1}$	8.301721×10^{-1}	7.911222×10^{-1}	7.776999×10^{-1}	7.708110×10^{-1}	$\mathcal{E}_{r_{1,s}}$	$2.884750 \times 10^{+1}$	$4.667223 \times 10^{+1}$	$6.029605 \times 10^{+1}$	$8.043906 \times 10^{+1}$	$1.075049 \times 10^{+2}$	$1.467492 \times 10^{+2}$
\mathcal{E}_T	$1.652013 \times 10^{+1}$	2.080172	2.041122	2.027700	2.020811	\mathcal{E}_T	$3.994781 \times 10^{+1}$	$6.147019 \times 10^{+1}$	$7.693777 \times 10^{+1}$	$1.026287 \times 10^{+2}$	$1.341154 \times 10^{+2}$	$1.799804 \times 10^{+2}$
\mathcal{E}_3^B	5.709501	1.289070	1.270287	1.263724	1.260334	\mathcal{E}_3^B	$1.901295 \times 10^{+1}$	$2.302225 \times 10^{+1}$	$2.449500 \times 10^{+1}$	$4.497582 \times 10^{+1}$	$5.025829 \times 10^{+1}$	$7.525961 \times 10^{+1}$
\mathcal{E}_2^B	5.709501	1.289070	1.270287	1.263724	1.260334	\mathcal{E}_2^B	$1.901295 \times 10^{+1}$	$3.356167 \times 10^{+1}$	$4.555195 \times 10^{+1}$	$4.497582 \times 10^{+1}$	$6.497626 \times 10^{+1}$	$7.525961 \times 10^{+1}$
$\langle r \rangle$	2.684659	2.684659	2.684659	2.684659	2.684659	$\langle r \rangle$	3.023182×10^{-1}	2.267761×10^{-1}	2.016512×10^{-1}	1.512341×10^{-1}	1.261092×10^{-1}	1.009842×10^{-1}
$\langle Q \rangle$	5.085355	5.089840×10^{-1}	3.687731×10^{-1}	3.039323×10^{-1}	2.640187×10^{-1}	$\langle Q \rangle$	2.573040×10^{-1}	2.022886×10^{-1}	1.779739×10^{-1}	1.540874×10^{-1}	1.332866×10^{-1}	1.140809×10^{-1}
						n_r	5	6	6	7	8	9
						W_r	$7.809046 \times 10^{+1}$	$8.464026 \times 10^{+1}$	$1.070459 \times 10^{+2}$	$1.245592 \times 10^{+2}$	$1.236029 \times 10^{+2}$	$1.385771 \times 10^{+2}$
						\mathcal{E}_r^K	3.931354×10^{-2}	3.162311×10^{-2}	3.556322×10^{-2}	3.079873×10^{-2}	2.533865×10^{-2}	2.264663×10^{-2}
						\mathcal{E}_r^R	3.161700×10^{-1}	3.036170×10^{-1}	3.414465×10^{-1}	3.435360×10^{-1}	3.218995×10^{-1}	3.227438×10^{-1}
						\mathcal{E}_r^C	1.973985×10^{-1}	1.834316×10^{-1}	2.062865×10^{-1}	2.025667×10^{-1}	1.862884×10^{-1}	1.840185×10^{-1}
						\mathcal{E}_r	5.528821×10^{-1}	5.186717×10^{-1}	5.832962×10^{-1}	5.769015×10^{-1}	5.335266×10^{-1}	5.294090×10^{-1}
						$\mathcal{E}_{r_{1,s}}$	5.526275×10^{-1}	5.452907×10^{-1}	7.044633×10^{-1}	6.150924×10^{-1}	5.672157×10^{-1}	5.566371×10^{-1}
						\mathcal{E}_T	1.105510	1.063962	1.287759	1.191994	1.100742	1.086046
						\mathcal{E}_3^B	7.044635×10^{-1}	6.147595×10^{-1}	6.750492×10^{-1}	7.511407×10^{-1}	6.582968×10^{-1}	6.888278×10^{-1}
						\mathcal{E}_2^B	7.044635×10^{-1}	7.378958×10^{-1}	9.210662×10^{-1}	7.511407×10^{-1}	7.359516×10^{-1}	6.888278×10^{-1}
						$\langle r \rangle$	3.399547	3.504126	3.115897	3.073171	3.260075	3.235919
						$\langle Q \rangle$	1.859022	1.871486	1.646537	1.762100	1.834960	1.852314
						$\langle r \rangle_{Coul}$	3.299486[57]	3.100710[57]	3.036524[57]	2.834452[57]	2.747914[57]	2.652825[57]

TABLE IV. Hookean model results for three-body antiprotonic systems (atoms and molecules). Data in muonic units.

Atom	$e^+p^-p^-$	$p^+p^-p^-$	$d^+p^-p^-$	$t^+p^-p^-$	$he^{+2}p^-p^-$	
n_r	1	1	1	1	1	
W_r	$4.076371 \times 10^{+3}$	$4.076371 \times 10^{+3}$	$4.076371 \times 10^{+3}$	$4.076371 \times 10^{+3}$	$4.076371 \times 10^{+3}$	
\mathcal{E}_r^K	2.570099	2.570099	2.570099	2.570099	2.570099	
\mathcal{E}_r^R	3.973405	3.973405	3.973405	3.973405	3.973405	
\mathcal{E}_r^C	4.556802	4.556802	4.556802	4.556802	4.556802	
\mathcal{E}_r	$1.110031 \times 10^{+1}$	$1.110031 \times 10^{+1}$	$1.110031 \times 10^{+1}$	$1.110031 \times 10^{+1}$	$1.110031 \times 10^{+1}$	
\mathcal{E}_{r1s}	$4.036591 \times 10^{+2}$	$1.153578 \times 10^{+1}$	9.420091	8.601868	8.156089	
\mathcal{E}_T	$4.147594 \times 10^{+2}$	$2.263608 \times 10^{+1}$	$2.052040 \times 10^{+1}$	$1.970217 \times 10^{+1}$	$1.925639 \times 10^{+1}$	
\mathcal{E}_3^B	$1.292905 \times 10^{+2}$	$1.321716 \times 10^{+1}$	$1.236270 \times 10^{+1}$	$1.200964 \times 10^{+1}$	$1.181060 \times 10^{+1}$	
\mathcal{E}_2^B	$1.292905 \times 10^{+2}$	$1.321716 \times 10^{+1}$	$1.236270 \times 10^{+1}$	$1.200964 \times 10^{+1}$	$1.181060 \times 10^{+1}$	
$\langle r \rangle$	3.023182×10^{-1}	3.023182×10^{-1}	3.023182×10^{-1}	3.023182×10^{-1}	3.023182×10^{-1}	
$\langle Q \rangle$	9.890888×10^{-1}	1.365415×10^{-1}	1.068694×10^{-1}	9.138743×10^{-2}	8.116479×10^{-2}	
Molecule	$p^-p^+p^+$	$p^-d^+p^+$	$p^-t^+p^+$	$p^-d^+d^+$	$p^-t^+d^+$	$p^-t^+t^+$
n_r	1	1	1	1	1	1
W_r	$4.076371 \times 10^{+3}$	$7.244484 \times 10^{+3}$	$9.162218 \times 10^{+3}$	$1.628931 \times 10^{+4}$	$2.342658 \times 10^{+4}$	$3.653383 \times 10^{+4}$
\mathcal{E}_r^K	2.570099	3.426232	3.853127	5.137647	6.161230	7.694149
\mathcal{E}_r^R	3.973405	5.296997	5.956982	7.942866	9.525338	$1.189525 \times 10^{+1}$
\mathcal{E}_r^C	4.556802	6.074730	6.831618	9.109080	$1.092390 \times 10^{+1}$	$1.364177 \times 10^{+1}$
\mathcal{E}_r	$1.110031 \times 10^{+1}$	$1.479796 \times 10^{+1}$	$1.664173 \times 10^{+1}$	$2.218959 \times 10^{+1}$	$2.661047 \times 10^{+1}$	$3.323117 \times 10^{+1}$
\mathcal{E}_{r1s}	$1.153578 \times 10^{+1}$	$1.775535 \times 10^{+1}$	$2.231319 \times 10^{+1}$	$2.976455 \times 10^{+1}$	$3.908552 \times 10^{+1}$	$5.270548 \times 10^{+1}$
\mathcal{E}_T	$2.263608 \times 10^{+1}$	$3.255331 \times 10^{+1}$	$3.895491 \times 10^{+1}$	$5.195415 \times 10^{+1}$	$6.569599 \times 10^{+1}$	$8.593666 \times 10^{+1}$
\mathcal{E}_3^B	$1.321716 \times 10^{+1}$	$1.717736 \times 10^{+1}$	$1.900053 \times 10^{+1}$	$2.889786 \times 10^{+1}$	$3.378852 \times 10^{+1}$	$4.609058 \times 10^{+1}$
\mathcal{E}_2^B	$1.321716 \times 10^{+1}$	$1.999682 \times 10^{+1}$	$2.483394 \times 10^{+1}$	$2.889786 \times 10^{+1}$	$3.804615 \times 10^{+1}$	$4.609058 \times 10^{+1}$
$\langle r \rangle$	3.023182×10^{-1}	2.267761×10^{-1}	2.016512×10^{-1}	1.512341×10^{-1}	1.261092×10^{-1}	1.009842×10^{-1}
$\langle Q \rangle$	1.365415×10^{-1}	1.100585×10^{-1}	9.817647×10^{-2}	8.500384×10^{-2}	7.417888×10^{-2}	6.387933×10^{-2}
n_r				10	12	12
W_r				$4.590259 \times 10^{+1}$	$3.931810 \times 10^{+1}$	$6.131671 \times 10^{+1}$
\mathcal{E}_r^K				1.119390×10^{-2}	7.952041×10^{-3}	9.930515×10^{-3}
\mathcal{E}_r^R				1.768315×10^{-1}	1.501797×10^{-1}	1.875446×10^{-1}
\mathcal{E}_r^C				9.960965×10^{-2}	8.304190×10^{-2}	1.037028×10^{-1}
\mathcal{E}_r				2.876350×10^{-1}	2.411737×10^{-1}	3.011779×10^{-1}
\mathcal{E}_{r1s}				8.387528×10^{-2}	6.559935×10^{-2}	8.845847×10^{-2}
\mathcal{E}_T				3.715103×10^{-1}	3.067730×10^{-1}	3.896363×10^{-1}
\mathcal{E}_3^B				3.065387×10^{-1}	2.532210×10^{-1}	3.227605×10^{-1}
\mathcal{E}_2^B				3.065387×10^{-1}	2.603668×10^{-1}	3.227605×10^{-1}
$\langle r \rangle$				5.882775	6.884813	5.513139
$\langle Q \rangle$				1.601295	1.810666	1.559260
$\langle r \rangle_{Coul}$				5.797779[57]	6.533299[57]	4.794814[57]

lently of the applied external magnetic field). However, Yannouleas and Landman [97] have reinterpreted these results as a prototypical three-body problem corresponding to a linear molecule XYX where the X 's are the electrons and the Y an infinitely heavy confining dot. Through this interpretation the rovibration nature of the two-electron quantum dot spectra is revealed.

The Hamiltonian for a two-electron three-dimensional quantum dot in a magnetic field ($\mathbf{B} \parallel z$) described by the vector potential $\mathbf{A} = (-y, x, 0)\mathbf{B}/2$, is:

$$\hat{H} = \sum_{j=1}^2 \left\{ \frac{1}{2m^*} (\mathbf{P}_j - e\mathbf{A}_j)^2 + \frac{m^*}{2} [w_o^2(x_j^2 + y_j^2) + w_z^2 z_j^2] \right\} + \frac{e^2}{4\pi\epsilon_0\epsilon} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (51)$$

(where m^* is the effective mass and ϵ an effective dielectric constant). This Hamiltonian separates in relative and center-of-mass coordinates $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, respectively, into

TABLE V. Hookean model results for “exotic” three-body pionic molecular systems [57]. Data in muonic units.

Molecule	$\mu^- \pi^+ \pi^+$	$\pi^- \mu^+ \mu^+$	$\mu^- \mu^+ \pi^+$	$\pi^- \mu^+ \pi^+$
n_r	1	1	1	1
W_r	$9.019558 \times 10^{+1}$	$5.169207 \times 10^{+1}$	$6.697615 \times 10^{+1}$	$6.697615 \times 10^{+1}$
\mathcal{E}_r^K	3.823012×10^{-1}	2.894176×10^{-1}	3.294375×10^{-1}	3.294375×10^{-1}
\mathcal{E}_r^R	5.910423×10^{-1}	4.474432×10^{-1}	5.093145×10^{-1}	5.093145×10^{-1}
\mathcal{E}_r^C	6.778223×10^{-1}	5.131392×10^{-1}	5.840948×10^{-1}	5.840948×10^{-1}
\mathcal{E}_r	1.651166	1.250000	1.422847	1.422847
\mathcal{E}_{r1s}	1.890618	1.189189	1.555749	1.417526
\mathcal{E}_T	3.541784	2.439189	2.978595	2.840373
\mathcal{E}_3^B	2.032492	1.445039	1.771270	1.708753
\mathcal{E}_2^B	2.032492	1.445039	1.678005	1.633047
$\langle r \rangle$	2.032397	2.684659	2.358528	2.358528
$\langle Q \rangle$	1.005076	1.102643	1.107978	1.009938
n_r	3	3	4	4
W_r	6.591000	3.777373	2.323564	2.323564
\mathcal{E}_r^K	2.330221×10^{-2}	1.764072×10^{-2}	9.274569×10^{-3}	9.274569×10^{-3}
\mathcal{E}_r^R	1.137202×10^{-1}	8.609083×10^{-2}	6.003148×10^{-2}	6.003148×10^{-2}
\mathcal{E}_r^C	8.016230×10^{-2}	6.068614×10^{-2}	3.929031×10^{-2}	3.929031×10^{-2}
\mathcal{E}_r	2.171847×10^{-1}	1.644177×10^{-1}	1.085964×10^{-1}	1.085964×10^{-1}
\mathcal{E}_{r1s}	1.381561×10^{-1}	8.689944×10^{-2}	5.397266×10^{-2}	4.917738×10^{-2}
\mathcal{E}_T	3.553408×10^{-1}	2.513171×10^{-1}	1.625690×10^{-1}	1.577737×10^{-1}
\mathcal{E}_3^B	2.450500×10^{-1}	1.786700×10^{-1}	1.206840×10^{-1}	1.185151×10^{-1}
\mathcal{E}_2^B	2.450500×10^{-1}	1.786700×10^{-1}	1.174484×10^{-1}	1.158887×10^{-1}
$\langle r \rangle$	9.784136	$1.292418 \times 10^{+1}$	$1.815900 \times 10^{+1}$	$1.815900 \times 10^{+1}$
$\langle Q \rangle$	3.718054	4.078983	5.948586	5.422226
$\langle r \rangle_{Coul}$	7.249287[57]	7.714412[57]	13.205[57]	17.100[57]

$$\hat{H}_r = -\nabla_r^2 + \gamma^2 r^2 + \frac{1}{r} + \frac{\hbar^* w_0}{2} t \left(i \frac{\partial}{\partial \varphi_r} \right) \quad (52)$$

$$\mathcal{E}'' = \frac{1}{2} \mathcal{E}' - \frac{\hbar^* \omega_0}{4} t m_r. \quad (57)$$

and

$$\hat{H}_R = -\frac{1}{4} \nabla_R^2 + 4\gamma^2 R^2 + \frac{\hbar^* w_0}{2} t \left(i \frac{\partial}{\partial \varphi_R} \right). \quad (53)$$

Here we have defined

$$\gamma^2 \equiv \left(\frac{\hbar^* w_0}{2} \right)^2 \left(\frac{t^2}{4} + 1 \right), \quad (54)$$

where $t = \omega_C / \omega_0$, $\omega_C = eB / m^*$. The confinement strength on the z axis has been set to:

$$\omega_z^2 = \omega_0^2 + \left(\frac{eB}{2m^*} \right)^2. \quad (55)$$

Recall that $\hbar^* = \hbar / \mathcal{E}_h$, with \mathcal{E}_h being the Hartree energy. From Eq. (52) we obtain the radial equation:

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} + \frac{1}{2} \frac{l_r(l_r+1)}{r^2} + \frac{\gamma^2}{2} r^2 + \frac{1}{2r} \right] u(r) = \mathcal{E}'' u(r) \quad (56)$$

with

Observe that Eq. (56) is of the same type as Eq. (32), whose eigenenergies are given by Eq. (34) for the discrete set of values of $\gamma = W_r(n_r, l_r)$ which afford an analytical close form solution. Consequently, from Eqs. (34) and (57) the energy of the two-electron quantum dot in a magnetic field ($\mathbf{B}||z$) is given by

$$\mathcal{E}' = 2W_r(n_r, l_r) \left(n_r + l_r + \frac{3}{2} \right) + \frac{\hbar^* w_0}{2} t m_r. \quad (58)$$

As mentioned above, Eq. (56) is exactly soluble [43,93] only for a discrete set of values of the coupling constant $\gamma = W_r(n_r, l_r)$. These values, for a given l_r , starting from $W_r(1, l_r)$ decrease for $n_r > 1$. Also, for values of $\gamma > W_r(1, l_r)$ we can calculate accurate energies for each l_r by taking the uncorrelated solution (with $n_r = 0$) of Eq. (33) and correcting it for the electronic interaction in first order of perturbation theory (this is allowed in this case as we are in the weakly correlated regime). We have used both the exact values of the energy for the points where $\gamma = W_r(n_r, l_r)$ plus some approximate values of the energy [calculated at a few points for $\gamma > W_r(1, l_r)$] to interpolate the energy of the quantum dot for arbitrary coupling constant (cf. [93]). The result-

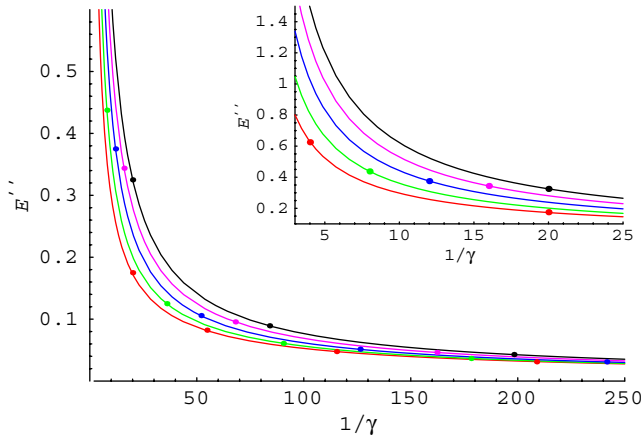


FIG. 1. (Color online) Energy of Eq. (57) of a two-electron three-dimensional quantum dot interpolated in a wide range values of γ for $l_r=0-4$. Curves run in order from bottom, $l_r=0$, to top $l_r=4$. (Color: $l_r=0$ red curve, $l_r=1$ green curve, $l_r=2$, blue curve, $l_r=3$ magenta curve and, $l_r=4$ black curve.) Inset: Detailed view for the most sensible values of γ .

ing energies plotted vs $1/\gamma$ are given in Fig. 1 for $l_r=0$ to $l_r=4$.

Now we can reconstruct the total energy \mathcal{E}' for arbitrary values γ , and not only for those $\gamma=W_r$ which enable an analytical solution of Eq. (56). Thus, Fig. 2 shows the energy of the two-electron three-dimensional quantum dot as a function of $t=eB/m^*\omega_0$. Observe that when the azimuth quantum number $m_r=0$ the energy curves corresponding to various values of l_r do not cross but, for the minimum energy states, i.e.: $m_r=-l_r$, they do cross. Since, the polar quantum number l_r conveys the spin state of the total wave function, namely, for l_r even the state must be singlet and for odd values of l_r the state must be triplet; Fig. 3 reveals that singlet-triplet and triplet-singlet transitions take place as the external magnetic field ($\mathbf{B}\parallel z$) increases. This behavior has recently been observed experimentally for two-electron two-dimensional quantum dots [63]. We predict that it should also be seen in two-electron three-dimensional quantum dots.

The exact solutions given by Eq. (33) depend on $n_r=0,1,2,\dots$ which is not exactly a quantum number but rather a parameter which describes the order of the correlation polynomial of Eq. (33). In this sense, n_r defines the degree of interelectronic correlation. For decreasing values

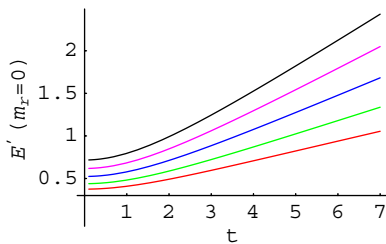


FIG. 2. (Color online) Energy of a two-electron three-dimensional quantum dot as a function of $t=eB/m^*\omega_0$ for $m_r=0$ and $l_r=0-4$. Curves run in order from bottom, $l_r=0$, to top $l_r=4$. (Color: $l_r=0$ red curve, $l_r=1$ green curve, $l_r=2$, blue curve, $l_r=3$ magenta curve and, $l_r=4$ black curve.)

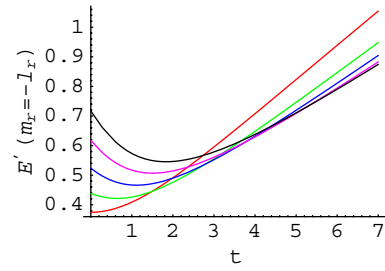


FIG. 3. (Color online) Ground states energy ($m_r=-l_r$) of a two-electron three-dimensional quantum dot as a function of $t=eB/m^*\omega_0$ for $l_r=0-4$. Curves run in order at $t=0$ from bottom, $l_r=0$, to top $l_r=4$. (Color: $l_r=0$ red curve, $l_r=1$ green curve, $l_r=2$, blue curve, $l_r=3$ magenta curve and, $l_r=4$ black curve.)

of the coupling constant, we observe higher values of the correlation parameter, denoting a more structured type of correlation (a higher order polynomial). A heuristic noninteger parameter n_r^* may be introduced assuming that for all values of γ [and not only those for which $\gamma=W_r(n_r, l_r)$] an equation of the type

$$\mathcal{E}' = 2\gamma\left(n_r^* + l_r + \frac{3}{2}\right) + \frac{\hbar^* w_0}{2} t m_r \quad (59)$$

holds. In Fig. 4 we plot n_r^* vs $\ln \gamma$.

As mentioned above, Yannouleas and Landman [97] have suggested a more elaborate model for a two-electron quantum dot, where the electrons [described by the Hamiltonian (16)] couple their motion to that of an infinite mass representing the quantum dot. In order to establish a connection with Yannouleas and Landman's XYX model, we consider the effect on the three-body system of taking the limit when the mass m_1 goes to infinity. From Eq. (24), using Eqs. (7) and (22), one can straightforwardly obtain

$$\mathbf{P} = \frac{\sqrt{m_1}}{\sqrt{M_{123}}} \mathbf{r}_1 + \frac{m_2}{\sqrt{m_1}} \frac{1}{\sqrt{M_{123}}} \mathbf{r}_2 + \frac{m_3}{\sqrt{m_1}} \frac{1}{\sqrt{M_{123}}} \mathbf{r}_3, \quad (60)$$

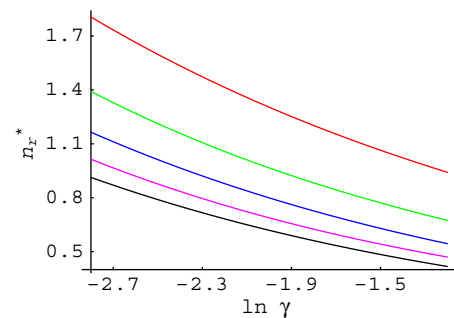


FIG. 4. (Color online) Effective radial quantum number of a two-electron three-dimensional quantum dot as a function of γ for $l_r=0-4$. Curves run in order from top, $l_r=0$, to bottom $l_r=4$. (Color: $l_r=0$ red curve, $l_r=1$ green curve, $l_r=2$, blue curve, $l_r=3$ magenta curve and, $l_r=4$ black curve.)

$$\mathbf{Q} = -\frac{\sqrt{M_{23}}}{\sqrt{M_{123}}}\mathbf{r}_1 + \frac{m_2}{\sqrt{M_{23}}}\frac{1}{\sqrt{M_{123}}}\mathbf{r}_2 + \frac{m_3}{\sqrt{M_{23}}}\frac{1}{\sqrt{M_{123}}}\mathbf{r}_3 \quad (61)$$

and taking $m_1 \rightarrow \infty$ it is seen that

$$\lim_{m_1 \rightarrow \infty} \mathbf{P} = \mathbf{r}_1, \quad (62)$$

$$\lim_{m_1 \rightarrow \infty} \mathbf{Q} = \mathbf{0}. \quad (63)$$

Setting $\mathbf{Q}=\mathbf{0}$ in Eq. (61) and identifying $m_2=m_3=m_e$ we obtain $\mathbf{r}_1=(\mathbf{r}_2+\mathbf{r}_3)/2$. Thus, \mathbf{r}_1 coincides with the coordinate \mathbf{R} of the center-of-mass motion in Eq. (53). Placing the center of coordinates in the position of the infinitely massive particle m_1 is, hence, equivalent to selecting the center-of-mass coordinate as the origin. In this case, from $\mathbf{r}_1=\mathbf{R}=\mathbf{0}$, it follows that $\mathbf{r}_2=-\mathbf{r}_3$. In turn, this result implies that for infinite m_1 the electrons move on the opposite sides of a rotating sphere. From this we conclude that in the infinite mass limit motion of the electrons in a quantum dot is that of a rigid rotator XYX , which is equivalent to a collectively rotating Wigner molecule [98–100].

However, when the mass $m_1 \gg m_e$ is finite, the coordinate \mathbf{P} (which in the three-body problem considered here is proportional to the center of mass) is slightly displaced from the position \mathbf{r}_1 of the more massive particle m_1 . Similarly, since the collective coordinate \mathbf{Q} is different from zero, for any value of \mathbf{Q} there arises a functional dependency between the coordinate \mathbf{r}_1 and that of the center-of-mass motion of the electrons. Since the motion of \mathbf{Q} is governed by an equation of a three-dimensional harmonic oscillator (27), it has characteristic vibrations and rotations. However, from Eq. (61) it is clear that the vibrations arise from a coupling of the motions of the coordinate of the massive particle (\mathbf{r}_1) with that of the center of mass of the electrons. This motion, therefore, may be described as that of a “floppy” system. Hence, the present three-body model leads us to the same type of conclusions already advanced by Yannouleas and Landman [97]. Moreover, since the value of W_Q given by Eq. (28) depends both on the relative mass $M=(m_2+m_3)/m_1$ and also on the parameter ω which effectively defines the steepness of the confining potential of the quantum dot, we may conclude that the degree of floppiness and its effect on the spectra [97] could be possibly controlled through variations of these parameters [101].

Impurities have been long recognized as important elements in spherical quantum dot systems (see, for example [102] and references therein). Depending on their type and location, they are able to induce symmetry breaking leading to the formation of Wigner molecules [103]. The presence of an impurity with mass m_1 and charge Z_1 converts the two-body problem given by Eq. (51) into a proper three-body problem. Clearly, the impurity contributes to the Hamiltonian (51) with an additional kinetic energy term plus two other terms arising from the Coulomb interaction between the charged impurity and the pair of electrons. However, in the effective mass regime, the effect of the impurity is incorporated solely via the additional Coulomb interaction [103].

The prototypical three-body system considered in the present work, may be regarded as a model for impurities in quantum dots provided the Coulombic interactions in the latter are replaced by harmonic ones. In this approximation, the results of the three-body problem obtained here are directly applicable to the description of an impurity of mass m_1 placed at the position \mathbf{r}_1 in a two-electron quantum dot. For finite mass m_1 , the energy spectrum is modified according to Eq. (49).

VI. DISCUSSION

The following observations are in order with respect to the Hookean model for the three-body problem that we have considered here.

In the first place, the adoption of a Hookean type interaction between the positive and negative particles is not sufficient to guarantee decoupling in the case where the particles with the same charge have different masses. Decoupling occurs only when the condition relating force constants and masses given by Eq. (13) is satisfied.

In the second place, we observe that the $n_r=1$ values of the quantum number determining the degree of the correlation polynomial for the interaction of particles with the same charge leads to Hookean systems with high energies and small values for the average of the interparticle distance as compared to the actual values for Coulomb systems. In order to have a more realistic approximation to the latter it is necessary to go to higher values of n_r . For electron-positron systems $\text{Ps}^-(e^+e^-e^-)$ the actual value of $\langle r \rangle_{\text{Coul}}=8.55$ (see Table I) is bracketed between $n_r=2$ and $n_r=3$. For $\text{H}^-(p^+e^-e^-)$, between $n_r=1$ and $n_r=2$. However, for the Hookean finite mass helium atom ${}^4\text{He}$ the bracketing occurs between $n_r=0$ and $n_r=1$. From the above observations we may infer that the electrons in Ps^- are more correlated than those in H^- and the latter, more so than those in ${}^4\text{He}$. Moreover, it is clear that the analytic functions obtained as discrete solutions to the Hookean problem do not exactly correspond to those solution that best represent the distance $\langle r \rangle_{\text{Coul}}$ for Coulomb systems.

In the third place, we observe that for massive particles with the same charge, it is necessary to go to extremely high n_r values ($n_r=65$ for H_2^+ and $n_r=75$ for HD^+). These results are in agreement with the values found for the nuclei interparticle distance for the Hookean model of the diatomic molecule H_2 [58]. Again, we find that it is the nature of the correlation function between the nuclei the determining factor in their spatial localization. As observed previously, this behavior fits the pattern of Wigner crystallization. This is attested in the present case by noticing from Table II that the ratio of the kinetic energy \mathcal{E}_r^K to the interparticle energy \mathcal{E}_r goes from 0.23 for $n_r=1$ to 0.007 for $n_r=65$ in H_2^+ , for example. The same behavior is observed for HD^+ (Table II) as well as for the muonic molecules reported in Table III, the antiprotonic ones, in Table IV and the exotic (pionic) ones, in Table V. However, it is clear that for muonic, antiprotonic, and pionic systems, the suitable values for n_r are considerably lower than those for the electronic molecules H_2^+ and HD^+ . The reason, of course, stems from the fact that in the

latter, the relation between masses is less pronounced than in the former.

The above considerations lead us to conclude that since for each one of these higher values of n_r (i.e., $n_r > 1$) we select the nodeless wave function (i.e., the wave function that complies with the requirement of being a ground state), and since the energy corresponding to this wave function always lies below that of the ground state for $n_r = 1$, it is clear that we can find two excited states corresponding to the given $n_r > 1$ that bracket the ground state energy for $n_r = 1$. In this sense, the results for $n_r = 1$ listed in the tables may be given in terms of interpolations between the energies of these excited states. It follows then that the energy for the ($n_r = 1$ and nodeless) ground-state wave function for the H_2^+ Hookean system lies between the energies of two excited and node-possessing wave functions for $n_r = 65$.

Now in the case of quantum dots, application of the three-particle Hookean model to these systems results in the following nontrivial observations. The first, that the exact analytic solutions including correlation obtained for the former are directly transferable to the latter. Clearly, the availability of exact analytic closed-form wave functions provides a very useful tool for the direct analysis of correlation phenomena. The second, that the inclusion of a mass m_1 (attributable to the implicit mass of the quantum dot [97]) allows for a more complex description of electron dynamics in quantum dots in

terms of such notions as electron molecules (or collectively rotating Wigner molecules [98–100]). As shown above, in the limit of infinite mass m_1 , there arises a picture of rigidly rotating XYX conformation (with equal distances $X-Y$ and $Y-X$). In addition, for finite mass, one enters a dynamic regime of what is usually characterized as “floppy” motion. Hence, the present results for two-electron three-dimensional quantum dots, offer a different and perhaps profitable perspective for the elucidation of this type of problem.

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- [1] F. Calogero, *J. Phys. A* **36**, 7291 (2003).
 - [2] F. Calogero and J.-P. Francoise, A. Guillot, *J. Math. Phys.* **44**, 5159 (2003).
 - [3] F. Calogero, *Theor. Math. Phys.* **133**, 1445 (2002).
 - [4] F. Calogero, *J. Phys. A* **35**, 4429 (2002).
 - [5] F. Calogero, *J. Phys. A* **35**, 985 (2002).
 - [6] M. M. Sano, *J. Phys. A* **37**, 803 (2004).
 - [7] M. A. Almeida, A. López-Castillo, and T. J. Stuchi, *J. Phys. A* **36**, 4805 (2003).
 - [8] A. Chenciner and R. Montgomery, *Ann. Math.* **152**, 881 (2000).
 - [9] K. R. Meyer, *Trans. Am. Math. Soc.* **352**, 2283 (2000).
 - [10] A. Santander, J. Mahecha, and F. Pérez, *Few-Body Syst.* **22**, 37 (1997).
 - [11] M. Nakato, *Chaos, Solitons Fractals* **11**, 171 (2000).
 - [12] L. Jiménez-Lara and E. Piña, *J. Math. Phys.* **44**, 4078 (2003).
 - [13] A. Hylleraas, *Z. Phys.* **48**, 469 (1928).
 - [14] H. Feshbach and S. I. Rubinow, *Phys. Rev.* **98**, 188 (1955).
 - [15] V. Aquilanti, S. Cavalli, C. Coletti, D. Di Domenico, and G. Grossi, *Int. Rev. Phys. Chem.* **20**, 673 (2001).
 - [16] V. Aquilanti and S. Tonzani, *J. Chem. Phys.* **120**, 4066 (2004).
 - [17] A. G. Abrashkevich, M. S. Kaschiev, and S. I. Vinitzky, *J. Comput. Phys.* **163**, 328 (2000).
 - [18] X.-Y. Gu, B. Duan, and Z.-Q. Ma, *Int. J. Mod. Phys. E* **10**, 69 (2001).
 - [19] E. Nielsen, D. V. Fedorov, A. S. Jensen, and E. Garrido, *Phys. Rep.* **347**, 373 (2001).
 - [20] N. Barnea and V. Mandelzweig, *Phys. Rev. C* **49**, 2910 (1994).
 - [21] Z. Papp, *Few-Body Syst.* **24**, 263 (1998).
 - [22] V. V. Pupyshev, *Theor. Math. Phys.* **136**, 970 (2003).
 - [23] Z.-Q. Ma, *Found. Phys. Lett.* **12**, 561 (1999).
 - [24] V. Efimov, *Phys. Rev. C* **47**, 1876 (1993).
 - [25] Z.-Z. Ren and G.-O. Xu, *Commun. Theor. Phys.* **25**, 203 (1996).
 - [26] E. Nielsen, D. V. Fedorov, and A. S. Jensen, *J. Phys. B* **31**, 4085 (1998).
 - [27] L. L. Lohr and S. M. Blinder, *Phys. Rev. A* **69**, 064102 (2004).
 - [28] M. Salci, S. B. Levin, and N. Elander, *Phys. Rev. A* **69**, 044501 (2004).
 - [29] R. A. Sultanov and D. Guster, *J. Comput. Phys.* **192**, 231 (2003).
 - [30] A. S. Kadyrov and I. Bray, *Nucl. Phys. A* **684**, 669c (2001).
 - [31] A. V. Matveenko, *Hyperfine Interact.* **138**, 117 (2001).
 - [32] W. Bian, X. Zhao, and Y. Wang, *Chem. Phys.* **242**, 195 (1999).
 - [33] W. Bian and C. Deng, *Theor. Chem. Acc.* **98**, 110 (1997).
 - [34] D. Kiang and A. Niégawa, *Phys. Rev. A* **14**, 911 (1976).
 - [35] V. V. Pupyshev, *Phys. At. Nucl.* **66**, 61 (2003).
 - [36] Z. Yalcin, M. Aktas, and M. Simsek, *Int. J. Quantum Chem.* **76**, 618 (2000).
 - [37] N. R. Kestner and O. Sinanoglu, *Phys. Rev.* **128**, 2687 (1962).
 - [38] E. Santos, *A. R. Soc. Esp. Fis. y Quim.* **64**, 177 (1968).
 - [39] R. J. White and W. Byers Brown, *J. Chem. Phys.* **53**, 3869 (1970).
 - [40] J. M. Benson and W. Byers Brown, *J. Chem. Phys.* **53**, 3880 (1970).
 - [41] S. Kais, D. R. Herschbach, and R. D. Levine, *J. Chem. Phys.* **91**, 7791 (1989).
 - [42] S. Kais, D. R. Herschbach, N. C. Handy, C. W. Murray, and G.

- J. Laming, *J. Chem. Phys.* **99**, 417 (1993).
- [43] M. Taut, *Phys. Rev. A* **48**, 3561 (1993).
- [44] J. Cioslowski and K. Pernal, *J. Chem. Phys.* **113**, 8434 (2000).
- [45] J. Karkowski and L. Cyrnek, *Ann. Phys.* **13**, 181 (2004).
- [46] R. Pino and V. Mujica, *J. Phys. B* **31**, 4537 (1998).
- [47] M. Taut, K. Pernal, J. Cioslowski, and V. Staemmler, *J. Chem. Phys.* **118**, 4861 (2003).
- [48] A. M. Frolov and V. H. Smith, Jr., *Phys. Rev. A* **53**, 3853 (1996).
- [49] C. Schwartz, *Phys. Rev.* **123**, 1700 (1961).
- [50] F. E. Harris, *Adv. Quantum Chem.* **47**, 129 (2004).
- [51] D. B. Kinghorn and L. Adamowicz, *J. Chem. Phys.* **110**, 7166 (1999).
- [52] D. M. Bishop and L. M. Cheung, *Phys. Rev. A* **16**, 640 (1977).
- [53] D. M. Bishop and L. P. Cheung, *Int. J. Quantum Chem.* **15**, 517 (1979).
- [54] A. M. Frolov, *Phys. Rev. A* **60**, 2834 (1999).
- [55] J. Shertzer, *Phys. Rev. A* **54**, 365 (1996).
- [56] S. Bubin, E. Bednarz, and L. Adamowicz, *J. Chem. Phys.* **122**, 041102 (2005).
- [57] D. M. Bishop, A. M. Frolov, and V. H. Smith, Jr., *Phys. Rev. A* **51**, 3636 (1995).
- [58] E. V. Ludeña, X. Lopez, and J. M. Ugalde, *J. Chem. Phys.* **123**, 024102 (2005).
- [59] X. Peng, J. Wickham, and A. P. Alivisatos, *J. Am. Chem. Soc.* **120**, 5343 (1998).
- [60] X. Peng, L. Manna, W. Yang, J. Wickham, E. Scher, A. Kadavanch, and A. P. Alivisatos, *Nature (London)* **404**, 59 (2000).
- [61] *Nanostructure Physics and Fabrication*, edited by M. A. Reed and W. P. Kirk (Academic, Boston, 1989).
- [62] Ch. Sikorski and U. Merkt, *Phys. Rev. Lett.* **62**, 2164 (1989).
- [63] C. Ellenberger, T. Ihn, C. Yannouleas, U. Landman, K. Enslin, D. Driscoll, and A. C. Gossard, *Phys. Rev. Lett.* **96**, 126806 (2006).
- [64] R. C. Ashoori, H. L. Stormer, J. S. Weiner, L. N. Pfeiffer, K. W. Baldwin, and K. W. West, *Phys. Rev. Lett.* **71**, 613 (1993).
- [65] D. Pfannkuche and S. E. Ulloa, *Phys. Rev. Lett.* **74**, 1194 (1995).
- [66] M. Tews, *Ann. Phys.* **13**, 249 (2004).
- [67] P. S. Drouvelis, P. Schmelcher, and F. K. Diakonov, *Phys. Rev. B* **69**, 035333 (2004).
- [68] D. Heitmann, V. Gudmundsson, M. Hochgräfe, R. Krahne, and D. Pfannkuche, *Physica E (Amsterdam)* **14**, 37 (2002).
- [69] Y. E. Lozovik and S. Y. Volkov, *Phys. Solid State* **45**, 364 (2003).
- [70] P. L. McEuen, E. B. Foxman, J. Kinaret, U. Meirav, M. A. Kastner, N. S. Wingreen, and S. J. Wind, *Phys. Rev. B* **45**, 11419 (1992).
- [71] G. W. Bryant, *Phys. Rev. Lett.* **59**, 1140 (1987).
- [72] J. Jung and J. E. Alvarellos, *J. Chem. Phys.* **118**, 10825 (2003).
- [73] D. C. Thompson and A. Alavi, *Phys. Rev. B* **69**, 201302(R) (2004).
- [74] P. A. Maksym and T. Chakraborty, *Phys. Rev. B* **45**, 1947 (1992).
- [75] M. Wagner, U. Merkt, and A. V. Chaplik, *Phys. Rev. B* **45**, 1951 (1992).
- [76] J. M. Kinaret, Y. Meir, N. S. Wingreen, P. A. Lee, and X. G. Wen, *Phys. Rev. B* **46**, 4681 (1992).
- [77] P. Hawrylak, *Phys. Rev. Lett.* **71**, 3347 (1993).
- [78] D. Pfannkuche, V. Gudmundsson, and P. A. Maksym, *Phys. Rev. B* **47**, 2244 (1993).
- [79] S. R. Eric Yang, A. H. MacDonald, and M. M. Johnson, *Phys. Rev. Lett.* **71**, 3194 (1993).
- [80] J. J. Palacios, L. Martin-Moreno, G. Chiappe, E. Louis, and C. Tejedor, *Phys. Rev. B* **50**, 5760 (1994).
- [81] C. de C. Chamon and X. G. Wen, *Phys. Rev. B* **49**, 8227 (1994).
- [82] M. Fujito, A. Natori, and H. Yasunaga, *Phys. Rev. B* **53**, 9952 (1996).
- [83] C. Yannouleas and U. Landmann, *Phys. Rev. Lett.* **82**, 5325 (1999).
- [84] U. Merkt, J. Huser, and M. Wagner, *Phys. Rev. B* **43**, 7320 (1991).
- [85] A. Matulis and F. M. Peeters, *J. Phys.: Condens. Matter* **6**, 7751 (1994).
- [86] T. M. Henderson, K. Runge, and R. J. Bartlett, *Chem. Phys. Lett.* **337**, 138 (2001).
- [87] M. Macucci, K. Hess, and G. J. Iafrate, *Phys. Rev. B* **48**, 17354 (1993).
- [88] M. Koskinen, M. Manninen, and S. M. Reimann, *Phys. Rev. Lett.* **79**, 1389 (1997).
- [89] K. Hirose and N. S. Wingreen, *Phys. Rev. B* **59**, 4604 (1999).
- [90] M. Gattobigio, P. Capuzzi, M. Polini, R. Asgari, and M. P. Tosi, *Phys. Rev. B* **72**, 045306 (2005).
- [91] A. V. Filinov, M. Bonitz, and Yu. E. Lozovik, *Phys. Rev. Lett.* **86**, 3851 (2001).
- [92] N. F. Johnson and M. C. Payne, *Phys. Rev. Lett.* **67**, 1157 (1991).
- [93] M. Taut, *J. Phys. A* **27**, 1045 (1994). R. Pino and V. M. Villalba, *J. Phys.: Condens. Matter* **13**, 11651 (2001).
- [94] J.-L. Zhu, Z.-Q. Li, J.-Z. Yu, K. Ohno, and Y. Kawazoe, *Phys. Rev. B* **55**, 15819 (1997).
- [95] M. Dineykhani and R. G. Nazmitdinov, *Phys. Rev. B* **55**, 13707 (1997).
- [96] M. Taut, *J. Phys.: Condens. Matter* **12**, 3689 (2000).
- [97] C. Yannouleas and U. Landman, *Phys. Rev. Lett.* **85**, 1726 (2000).
- [98] C. Yannouleas and U. Landman, *Phys. Rev. B* **68**, 035325 (2003).
- [99] C. Yannouleas and U. Landman, *Phys. Rev. B* **68**, 035326 (2003).
- [100] C. Yannouleas and U. Landman, *Phys. Rev. B* **69**, 113306 (2004).
- [101] G. Parascandolo, G. Cantele, D. Ninno, and G. Iadonisi, *Phys. Rev. B* **68**, 245318 (2003).
- [102] J. L. Movilla and J. Planelles, *Comput. Phys. Commun.* **170**, 144 (2005).
- [103] C. Yannouleas and U. Landman, *Phys. Rev. B* **61**, 15895 (2000).