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## Exact Solution of the Three-Body Santilli-Shillady Model of the Hydrogen Molecule

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The conventional representation of the H<sub>2</sub> molecule characterizes a 4-body system due to the independence of the orbitals of the two valence electrons as requested by quantum chemistry, under which conditions no exact solution is possible. To overcome this problem, Santilli and Shillady introduced in 1999 a new model of the H<sub>2</sub>-molecule in which the two valence electrons are deeply bounded-correlated into a single quasi-particle they called isoelectronium that is permitted by the covering hadronic chemistry. They pointed out that their new H<sub>2</sub>-model is a restricted 3-body system that, as such, is expected to admit an exact solution and suggested independent studies for its identification due to its relevance, e.g., for other molecules. In 2000, Aringazin and Kucherenko did study the Santilli-Shillady restricted 3-body model of the H<sub>2</sub> molecules, but they presented a variational solution that, as such, is not exact. In any case, the latter approach produced significant deviations from experimental data, such as a 19.6% inter-nuclear distance greater than the experimental value. In this paper we present, apparently for the first time, an exact solution of the Santilli-Shillady restricted 3-body model of the Hydrogen molecule along the lines of its originators and show that it does indeed represent correctly all basic data. Intriguingly, our solution confirms that the orbital of the isoelectronium (referred to as its charge distribution around the nuclei) must be concentrated in a limited region of space given by the Santilli-Shillady oo-shaped orbits. Our exact solution is constructed by following the Ley-Koo solution to the Schrödinger equation for a confined hydrogen molecular ion, H<sub>2</sub><sup>+</sup>. We show that a confined model to the 3-body molecule reproduces the ground state curve as calculated by Kolos, Szalewics and Monkhorst with a precision up to the 4-th digit and a precision in the representation of the binding energy up to the 5-th digit.

### 1 Introduction

As it is well known, the conventional representation of the Hydrogen molecule characterizes a four-body system due to the independence of the orbitals of the two valence electrons as requested by quantum chemistry, under which conditions no exact solution is possible. To overcome this problem, R. M. Santilli and D. Shillady introduced in 1999 a new model of the H<sub>2</sub>-molecule [1, 2], in which the two valence electrons are deeply bounded-correlated into a single quasi-particle they called isoelectronium that is permitted by the covering hadronic chemistry [3a].

They pointed out that their new model of Hydrogen molecule is a restricted three-body system that, as such, is expected to admit an exact solution; they suggested to carry out independent studies for its identification due to its relevance, e.g., for other molecules. In 2000, Aringazin and Kucherenko [4] did study the Santilli-Shillady restricted three-body model of the Hydrogen molecule, but they presented a variational solution that, as such, is not exact. In any case, the latter approach produced significant deviations from experimental data, such as a 19.6% inter-nuclear distance greater than the experimental value.

In this paper we present, apparently for the first time, an exact solution of the Santilli-Shillady restricted three-body model of the Hydrogen molecule along the lines of its originators and show that it does indeed represent correctly all basic data. Intriguingly, our solution confirms that the orbital of the isoelectronium (referred to as its charge distribution around the nuclei) must be concentrated in a limited region of space given by the Santilli-Shillady oo-shaped orbits. Our exact solution is constructed by following the E. Ley-Koo and A. Cruz solution to the Schrödinger equation for a confined hydrogen molecular ion, H<sub>2</sub><sup>+</sup> [5]. We show that a confined model to the three-body molecule reproduces the ground state curve as calculated by Kolos, Szalewics and Monkhorst [6] with a precision up to the 4-th digit and a precision in the representation of the binding energy up to the 5-th digit.

The suggestion that a kind of correlated state of electrons is present while they surround in closed paths the nuclei stimulates the search of a complementary quantum mechanical approach. In addition, Pérez-Enríquez [7], while working on high-Tc superconductivity, found that by using a Möbius-type orbital for Cooper pairs, there is a structural parameter in perovskite type superconductors that correlates linearly

with the critical temperature. Other contributions to the discussion about correlation between electrons were presented by Taut [8] in 1999. He reported that a one-particle representation could apply to systems with high densities of charge, based upon a pair-correlation function and density of charge for a system of two electrons in an external potential.

In our approach as it has been mentioned, we use the idea of a system under confinement as worked by E. Ley-Koo and A. Cruz for the hydrogen molecular ion and by other authors for molecules under pressure [9, 10]. Besides, previous studies related to the present discussion concerning hydrogenic impurities and excitons in quantum dots have been carried out by our team and others [11, 12, 13].

The main features of the restricted three-body Santilli-Shillady model, we discuss here, are summarized in section 2; special attention is drawn to the isoelectronium proposal. In this section, we also compare the results from this model with a standard ground state energy curve calculated by Kolos, Szalewics and Monkhorst (KSM curve) [6]. In section 3, we describe how to calculate the exact solution to the three-body model including a spheroidal confinement and a defect of mass parameters in order to reproduce the standard KSM curve, using a variational calculation. Finally, in section 4, some conclusions are made with regard to the accuracy of our results.

## 2 Iso-chemical model of the hydrogen molecule

The point of departure of the iso-chemical model of the hydrogen molecule, presented for the first time in 1999 by Santilli and Shillady [1], resides in the fact that the distance between nuclei is large; hence, the force binding them together comes from the orbiting electrons. The main hypothesis of the model describes how the valence electrons become involved in a binding process when they are at very short distance giving rise to a new state or quasi-particle, called isoelectronium. This particle would be responsible for the stability of the molecule and would describe a oo-shaped orbit around the nuclei “in a similar way as a planet orbits around binary stars” [1].

This hydrogen molecule model is forbidden by quantum mechanics and quantum chemistry since the proximity of electrons creates a repulsive Coulomb force between them; however, the authors assume that this difficulty can be overruled by a non-Hamiltonian interaction based on the overlapping of wave packets associated with each electron. This force surmounts the electrostatic one and allows the quasi-particle formation. They affirm that “the attractive force coming from the deep wave-overlapping does not have an equivalent in quantum mechanics and requires the new theory” [1]. This is the reason to introduce the so called iso-mechanics and iso-chemistry theories as part of hadronic mechanics [3b].

Our approach, however, uses the isoelectronium hypo-

thesis and at the same time looks for a compatible state in the frame of quantum chemistry. We will show that there exists a state reproducing the ground state energy of the hydrogen molecule in the frame of the restricted three-body Santilli-Shillady model.

The two basic notions of hadronic chemistry that we need for understanding the iso-chemical model of the hydrogen molecule are:

- (a) Hadronic horizon. The hadronic horizon is a distance between electrons,  $r_c$ , which measures one femtometer ( $1 \text{ fm} = 10^{-15} \text{ m}$ ). Outside this range quantum chemistry applies and within it hadronic chemistry is valid;
- (b) The trigger, which is given by external (conventional) interactions, causes the identical electrons to move one toward the other and penetrate the hadronic horizon against Coulomb interaction (once inside the said horizon, the attractive hadronic force overcomes the repulsive Coulomb one), resulting in a bound state.

Santilli presented for the first time the hypothesis of a bound state between electrons in 1978 [3], while explaining the structure of a  $\pi^0$  meson as a hadronic bound state of one electron and one positron. Later, Animalou [14] and Animalou and Santilli [15] extended the model to consider the Cooper pair in superconductivity as a hadronic bound state of two identical electrons.

According to Santilli, in the case of  $\pi^0$  there is no need for a trigger because the involved particles have opposite charges. However, the existence of the Cooper pair requires a trigger, which Santilli and Animalou identified as the field of the copper ions. In the case of the hydrogen molecule, they conjecture that the trigger, constituted by the field between nuclei, is sufficiently intense (attractive for the electrons) enough to draw them together. They assume, essentially, that atom attraction is sufficient to cause the overlapping between wave packets, thus pushing electrons beyond the hadronic horizon.

### 2.1 Four-body Santilli-Shillady model

The iso-chemical model of the hydrogen molecule uses the conventional quantum model of the  $\text{H}_2$  subject to a non-unitary transformation for the condition  $r_c = r_{12}$ . This inter electronic distance is small given that the electrons are inside the hadronic horizon. After using this transformation, one can reduce the problem to an equation that uses a Hulthén potential, recalling that at short distances, this behaves like a Coulomb potential,

$$\left\{ -\frac{\hbar^2}{2\mu_1} \nabla_1^2 - \frac{\hbar^2}{2\mu_2} \nabla_2^2 - V_0 \frac{e^{-r_{12}/r_c}}{1 - e^{-r_{12}/r_c}} + \frac{e^2}{r_{12}} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R} \right\} |\hat{\psi}\rangle = E |\hat{\psi}\rangle. \quad (1)$$

As Santilli and Shillady affirm, this equation exhibits a new explicitly attractive force among neutral atoms of the

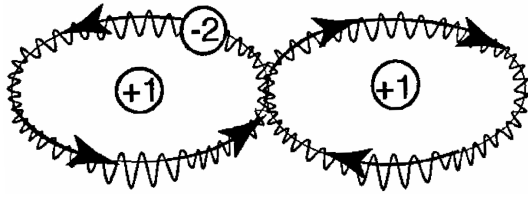


Fig. 1: Hydrogen molecule in the restricted three-body Santilli-Shillady model; a stable isoelectronium moves around nuclei in a oo-shaped orbit (figure taken from Santilli 1999, ref. [1]).

molecule in a way that is not possible within the quantum chemistry framework. They claim that Eq. (1) explains why only two hydrogen atoms make up the molecule and allows the exact representation of the binding energy in the full 4-body configuration.

A further simplification of the iso-chemical model can be introduced by making the two iso-electrons (electrons inside the hadronic horizon) be bound together into a state called isoelectronium as mentioned above. With this approximation, Equation (1) is reduced to a restricted three-body problem because one can consider  $r_{1a} \approx r_{2a} = r_a$  and  $r_{1b} \approx r_{2b} = r_b$  as  $r_{12} \ll r_a, r_b$ . In this manner, an exactly solvable problem similar to the conventional ion is obtained. One remarkable idea proposed by the authors consists in representing the isotopic model of the molecule as two H-protons at rest and the isoelectronium moving around them in a oo-shaped orbit, as it is shown in Figure 1 and described by the following structural equation:

$$\left\{ -\frac{\hbar^2}{2\mu_1} \nabla_1^2 - \frac{\hbar^2}{2\mu_2} \nabla_2^2 - V_0 \frac{e^{-r_{12}/r_c}}{1 - e^{-r_{12}/r_c}} + \frac{e^2}{r_{12}} - \frac{2e^2}{r_a} - \frac{2e^2}{r_b} + \frac{e^2}{R} \right\} |\hat{\psi}\rangle = E |\hat{\psi}\rangle. \quad (2)$$

This simplification, impossible in a quantum chemistry environment, could be used to reach an exact solution of the H-molecule. At this point, it is worth mentioning that with the aid of this model, Santilli and Shillady extended their analysis to other molecules; in particular, they studied the hydrogen and oxygen atoms in order to form HO. This gave them elements to present, for the first time, an exact solution to the water molecule, treated as an HOH molecule, using an isotopic intersection of an HO and an OH [2]. They have further their research to extend their model to another type of molecular chains and molecules.

Results for the Santilli-Shillady model of molecular hydrogen were obtained by the standard Boys-Reeves model [1], using an attractive Gaussian-screened-Coulomb potential. These authors used their SASLOBE programme (Santilli-Animalou-Shillady LOBE) to calculate the energies reported in columns three and four of Table 1, which in turn are compared with the quantum chemical results (first column).

Results from Table 1 show that the energy calculated by the SASLOBE program ( $-1.174444$  au) differs from the exact result in the 6th digit (a  $3 \times 10^{-5}$  error) with a 20 hours

Concept/species	H <sub>2</sub> <sup>a)</sup>	$\widehat{H}_2$ <sup>b)</sup>	$\widetilde{H}_2$ <sup>c)</sup>
Energy (variational)	-1.12822497	-7.61509174	*
Energy SCF (au)	1.14231305	*	-1.13291228
Energy SAS (au)	*	*	-1.174444
Energy exact <sup>d)</sup> (au)	-1.174474	*	-1.174474
Bond length (bohr)	1.4011	0.2592	1.4011
Isoelectronium radius (bohr)	*	*	0.01124995

Notes: <sup>a)</sup>Normal molecule in the quantum-chemical model  
<sup>b)</sup>Molecule in the restricted three-body model (see)  
<sup>c)</sup>Molecule in the iso-chemical model (stable isoelectronium)  
<sup>d)</sup>Ground state energy by Kolos, Szalewicz and Monhorst

Table 1: Comparison of results from Iso-chemical model. Taken from Santilli 1999, ref. [1].

process time in a 320 MFLOPS Silicon Graphics computer. Notice that some changes in the most expensive routines in the iso-chemical model improve by a factor of 1000 the time used to compute a Boys-Reeves C.I. calculation. An important result is that with their method, they found a bond length ( $R = 1.4011$  bohr) which coincides with that of the C.I. value.

This new way to represent chemical bonding has allowed the opening of a whole field named Hadronic Mechanics. With this new tool, several problems of physics and chemistry have been worked, leading to new proposals that range from energetic problems to superconductivity issues [16]. Our work has not taken that road; it considers the solution of the restricted three-body in the frame of Quantum Mechanics, two protons bound by an orbiting stable isoelectronium. This approach uses the solution of an  $H_2^+$  ion but with a charge  $q = -2e$  for the quasi-particle.

## 2.2 Restricted three-body Santilli-Shillady model

The four-body Santilli-Shillady model, as described by Eq. (2), was modified by Aringazin and Kucherenko [4] in order to restrict it to an explicit three-body approach. Within this restricted three-body Santilli-Shillady model (M3CS-S), these authors found a set of two equations that can be solved exactly. In this section we follow the main features of their method and show some of their results to contrast them with the results from our approach. The restricted Santilli-Shillady model assumes three basic conditions:

- A stable isoelectronium;
- The size of the isoelectronium can be neglected as compared with the inter nuclear distance; and,
- The Born-Oppenheimer approximation is valid.

When we combine these conditions with Eq. (2), representing a four-body equation, we arrive at a couple of differential equations which can be exactly solved. Aringazin and Kucherenko assumed that:

$$\mu_1 = \mu_2 = m_e. \quad (3)$$

And that the isoelectronium mass and reduced mass were

$$M = \mu_1 + \mu_2; \quad m = \frac{\mu_1 \mu_2}{M}. \quad (4)$$

In order to simplify expressions, they transformed the momentum operators

$$\bar{p}_i = -i\hbar \frac{\partial}{\partial r_i}, \quad i = 1, 2; \quad (5)$$

into generalized ones:

$$\bar{P}_M = -i\hbar \frac{\partial}{\partial \bar{r}_{ab}}, \quad \bar{p}_{12} = -i\hbar \frac{\partial}{\partial \bar{r}_{12}}. \quad (6)$$

Through them, Aringazin and his colleague arrived to a new equation from which the three-body equation can be derived by a variable separation method; i.e., from equation

$$\left\{ -\frac{\hbar^2}{2M} \nabla_{ab}^2 - \frac{\hbar^2}{2m} \nabla_{12}^2 - V_0 \frac{e^{-r_{12}/r_c}}{1 - e^{-r_{12}/r_c}} + \frac{e^2}{r_{12}} - \frac{2e^2}{r_a} - \frac{2e^2}{r_b} + \frac{e^2}{R} \right\} |\hat{\psi}\rangle = E |\hat{\psi}\rangle \quad (7)$$

they got two equations, one describing the electrons inside the hadronic horizon in terms of the distance between them:

$$-\frac{\hbar^2}{2m} \nabla_{12}^2 \chi + V(r_{12}) \chi = \varepsilon \chi; \quad (8)$$

and, the second for the isoelectronium interaction with the nuclei:

$$-\frac{\hbar^2}{2M} \nabla_{ab}^2 \psi + W(r_a, r_b, R) \psi = (E - \varepsilon) \psi, \quad (9)$$

where

$$|\hat{\psi}\rangle = \chi(r_{12}) \psi(r_a, r_b) \quad (10)$$

with

$$V(r_{12}) = \frac{e^2}{r_{12}} - V_0 \frac{e^{-r_{12}/r_c}}{1 - e^{-r_{12}/r_c}}, \quad (11)$$

and

$$W(r_a, r_b, R) = -\frac{2e^2}{r_a} - \frac{2e^2}{r_b} + \frac{e^2}{R}. \quad (12)$$

The Aringazin-Kucherenko proposal, Eqs. (9) and (12), becomes the restricted three-body Santilli-Shillady Model (M3CS-S) with which we are going to compare our results. On the other hand, Eqs. (8) and (11) become the description of the electrons involved in the isoelectronium itself. They have also considered that since the size of isoelectronium is small, the energy must be near zero,  $\varepsilon \approx 0$ ; a point we are not going to discuss here.

$\nu^a)$	$E$	$R_{opt}^b)$
0.3	-1.142556	1.722645
0.307	-1.169215	1.683367
0.308	-1.173024	1.677899
0.308381 <sup>c)</sup>	-1.174475	1.675828
0.309	-1.176832	1.672471

Notes: <sup>a)</sup>Mass parameter in

<sup>b)</sup>Optimum bond length (bohr)

<sup>c)</sup>Parameter to obtain best energy

Table 2: Minimum energy dependence on the mass parameter

The direct solution of these equations gives results for the energy and bond length far from the experimentally observed; for example, the minimum energy,  $E = -7.614289$  au, is much lower than  $E_e = -1.17447567$  au, while the bond length,  $R = 0.25$  bohr, markedly differs from  $R = 1.4011$  bohr.

### 2.3 Results from the Aringazin-Kucherenko approach

As it has just been mentioned, the application of the restricted three-body Santilli-Shillady model gives results far from the experimental values for both, energy and bond length. In order to correct this problem, Aringazin and his team have chosen a scaling method to equalize their energy value with that experimentally observed. By assuming a charge equal to  $-2e$  for the isoelectronium and its mass  $M = \nu m_e$ , they assigned to  $E$  the formula  $E = W + 1/R$  ( $W$  is isoelectronium energy) and  $R$  in Eq. (9) to get a scaling rule for their original calculated data. The summary of the scaling process is:

$$(R, W) \longrightarrow (R, W + 1/R) \longrightarrow \left( \frac{R}{2\nu}, 4\nu W \right) \longrightarrow \left( \frac{R}{2\nu}, 4\nu W + \frac{2\nu}{R} \right). \quad (13)$$

Values in Table 2 show energy variations with respect to mass parameter and allows the identification of  $\nu$  as the best parameter for the estimation of energy,  $E = -1.174475$  au. While we have a 7th significant digit precision to the desired energy, the correspondent bond length disagrees 19.6% from the expected value.

There are, in the literature, a great number of studies and estimates for the ground state energy of molecular hydrogen. This elemental molecule is the most studied one and has compelled researchers in this field to design tools and other quantum mechanical theories. To compare our results with those of Aringazin-Kucherenko, we are going to use as the ground state energy curve the values reported by Kolos, Szalewicz y Monkhorst [6] as reference. Though there are already other studies reporting higher precision values, up to 12 significant digits [17], for example, we will not employ them here for we do not need such precision as our method gives numbers up to the 6th significant digit. These data are going to be identified as Kolos data or KSM curve.

With the aid of the data for the electronic energy  $W$  as a function of the distance between nuclei in the molecule (we remit the reader to Table 2 in ref. [4]), it is possible to construct a curve for the molecular energy according to the M3CS-S model. In Figure 2, we present a graph comparing the corresponding curve with Kolos data. It is self evident that both curves are very different, mainly in the region  $R > 2.0$ , though profiles are similar for lower  $R$  values.

On the other hand, the optimum bond length,  $R = 1.675828$  bohr, of this curve is deviated from the experimentally observed value by 19.6%. These observations to the M3CS-S model imply that some kind of adjustment is

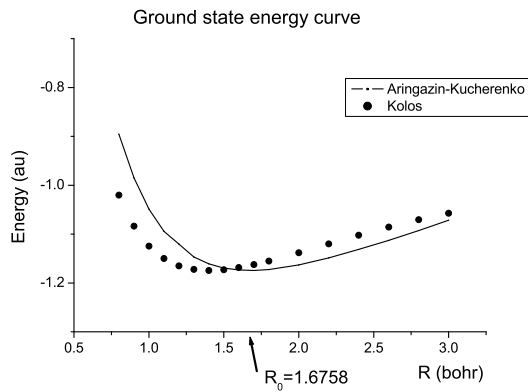


Fig. 2: Comparison between KSM's ground state energy data and scaled Aringazin-Kucherenko curve.

needed; probably a change in one of the features of the isoelectronium model could suppress these differences. In next section, we will present one such modification: the finite extension of isoelectronium.

### 3 Confined isoelectronium approach

We have shown until this point that the M3CS-S model satisfies the established conditions for the existence of isoelectronium with two drawbacks: it lacks the precision to represent the ground state potential energy curve of the hydrogen molecule and does not give a good approximation to its optimum bond length. In this section, we are going to introduce a condition directly related to the isoelectronium definition, a condition on the extension of isoelectronium wave function that will provide a modified three-body Santilli-Shillady model reproducing the behavior of the KSM curve in an appreciable range of distances between nuclei in the molecule.

The isoelectronium, as proposed by iso-chemistry, is a particle that brings together both electrons in the Hydrogen molecule, bound firmly (stable isoelectronium) by a Hulthén type potential. With a charge twice of the electron this quasi-particle has to orbit around protons in a very compact way. For an  $M = 2m_e$  particle, the results of the calculations give very low energies and small bond length values. From this picture, we consider that the four-body problem of the hydrogen molecule can be converted into a compatible three-body approach if some aspects of the quasi-particle formation and molecule structure are taken into account. First of all, the formation of particles involves the transformation of mass into energy as it is observed for example in nuclear reactions; this means that while electrons come together to form an isoelectronium, there must be an effective mass factor present in the description of the molecule. As seen from the Schrödinger equation, this parameter would appear as a scaling factor for the energy and bond length.

This kind of scaling has been suggested in the literature before, not just by Aringazin and Kucherenko but by other

authors as well. In particular, Svidzinsky and collaborators [18] have recently published a paper on the role of scaling while they attempt to represent the hydrogen molecule from Bohr's model. They make a dimensional scaling of the energy in this pre-quantum mechanical description. In our approach, scaling comes from an effective mass factor.

Another factor that must be considered in our model arises from the fact that a double charged particle surrounding both nuclei in the molecule can not extend in the same way as an electron does in the molecular ion. This small but heavily charged quasi-particle must have to limit its motion to confined orbits. Thus, the Hydrogen molecule with the isoelectronium orbiting two protons has to appear as a confined system. Therefore, as a way to improve the restricted three-body Santilli-Shillady model, a pair of conditions was introduced to understand the kind of movement an isoelectronium would describe. We have hypothesized the following additional restrictions for the isoelectronium model:

- The formation of the quasi-particle from the two electrons involves an effective mass transformation; i.e., the mass and charge of isoelectronium are  $M = \nu m_e$  and  $q = -2e$ , respectively, where  $\nu$  is the effective mass parameter, also called "iso-renormalization of mass"; and
- The spatial extension of the orbits of isoelectronium is limited to a defined region of space: the isoelectronium must orbit in a spheroidal shaped region of space.

Using these two hypotheses we have worked out two methods for the solution of the hydrogen molecule problem. First, the solution of Eq. (9) is considered in a way similar to the Ley-Koo and Cruz solution for the molecular ion confined by a spheroidal box [5]. They arrive to an exact solution for the differential equation by using separation of variables and the condition of a vanishing wave function on the spheroidal border. The second, whose results are reported here, uses a variational approach to solve Eq. (9) as it was done by Marín and Muñoz [19], with the same border condition:  $\psi(\xi_0, \eta, \varphi) = 0$  and  $\xi_0$  defines the shape of the box.

#### 3.1 Exact solution to the confined model

Our variational approach to solve the modified three-body Santilli-Shillady model of the hydrogen molecule (modified M3CS-S) arrives to the following equation after applying the Hamiltonian for  $H_2^+$ , but including the above stated conditions on the mass,  $M = \nu m_e$ , where  $\nu$  is the mass parameter, and the  $q = -2e$  is the charge:

$$\left\{ -\frac{\hbar}{2\nu m_e} \frac{4}{\rho^2 (\xi^2 - \eta^2)} \left[ \frac{\partial}{\partial \xi} (\xi^2 - 1) \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta} (1 - \eta^2) \frac{\partial}{\partial \eta} \right] + \frac{\xi^2 - \eta^2}{(\xi^2 - 1)(1 - \eta^2)} \frac{\partial^2}{\partial \varphi^2} - \frac{4e^2}{\rho} \frac{(Z_1 + Z_2)\xi + (Z_2 - Z_1)\eta}{\xi^2 - \eta^2} + \frac{Z_1 Z_2 e^2}{\rho} \right\} \psi(\xi, \eta, \varphi) = E' \psi(\xi, \eta, \varphi), \quad (14)$$

subject to the following restriction:

$$\psi(\xi_0, \eta, \varphi) = 0, \quad (15)$$

which specifies a spheroidal shaped region of space where the particle moves ( $\xi \leq \xi_0$ ). Moreover, the wave function must vanish at the border. Due to the symmetry of the molecule in the ground state ( $m = 0$ ), the azimuthal variable, can be suppressed so the problem is reduced to the  $z - x$  plane. In addition, we introduce atomic units:

$$a_0 = \frac{\hbar^2}{m_e e^2}; \quad E' = \frac{e^2}{2a_0} E; \quad R = \frac{\rho}{a_0}.$$

Thus, the equation is rewritten as

$$\tilde{H}\phi = E\phi$$

or

$$\left\{ -\frac{4}{\nu R^2(\xi^2 - \eta^2)} \left[ \frac{\partial}{\partial \xi}(\xi^2 - 1) \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta}(1 - \eta^2) \frac{\partial}{\partial \eta} \right] - \frac{8}{R} \frac{(Z_1 + Z_2)\xi + (Z_2 - Z_1)\eta}{\xi^2 - \eta^2} + \frac{Z_1 Z_2}{R} \right\} \phi(\xi, \eta) = E\phi(\xi, \eta). \quad (16)$$

With this reduction, the above stated conditions can be met by a simple variational function considering one parameter and a cut off factor:

$$\phi(\alpha; \xi, \eta) = (\xi_0 - \xi) \left( \exp[-\alpha(\xi + \eta)] + \exp[-\alpha(\xi - \eta)] \right). \quad (17)$$

The minimum energy of this modified M3CS-S molecule can be obtained by minimization of the functional of energy

$$E(\alpha) = \frac{\langle \phi | \tilde{H} | \phi \rangle}{\langle \phi | \phi \rangle} \quad (18)$$

subject to the condition

$$\left. \frac{\partial E}{\partial \alpha} \right|_{E=E_{\min}} = 0, \quad (19)$$

But really such a minimum energy,  $E_{\min}$ , will depend on several parameters

$$E_{\min} = E_{\min}(\nu, \xi_0, R), \quad (20)$$

i.e., mass scale, spheroidal box and nuclei separation parameters. If we leave free all three parameters and use a simplex optimization method, a Nelder-Mead method for example [20], we will find that this energy is located at a point near the one reported by Santilli-Shillady and included here in Table 1 ( $E = -7.61509174$  au and  $R = 0.2592$  bohr). However, we can choose a fixed value for the mass parameter and find the minimum energy suitable for the ground state energy of free  $H_2$ .

Effectively, in order to obtain the minimum energy corresponding to a given mass parameter,  $\nu$ , we have optimized the energy using the Nelder-Mead algorithm for two parameters:  $\xi_0$  — spheroidal box shape; and,  $R$  — bond length.

$\xi_0$ <sup>a)</sup>	$R$ <sup>b)</sup>	$\nu$ <sup>c)</sup>	$E$ <sup>d)</sup>
48.46714783	1.41847181	0.37030	-1.1741987
48.46714783	1.41847181	0.37035	-1.1743573
48.46714783	1.41847181	0.37038	-1.1744523
48.46714783	1.41847181	0.37039	-1.1744840 <sup>e)</sup>
48.46714783	1.41847181	0.37040	-1.1745157
48.46714783	1.41847181	0.37050	-1.1748325
48.46714783	1.41847181	0.37060	-1.1751492

Notes: <sup>a)</sup> Shape parameter inverse of eccentricity (optimization)  
<sup>b)</sup> Bond length parameter (optimization)  
<sup>c)</sup> Mass parameter up to five digits (fixed)  
<sup>d)</sup> Minimum energy (calculated by program)  
<sup>e)</sup> Nearest value to exact energy (error)

Table 3: Minimum energy from parameter optimization for the confined model.

One relevant aspect resulting from these calculations is that for all mass parameter values the convergence of the method yields always identical values for both parameters as can be seen in Table 3 ( $\xi_0 = 48.46714783$ ;  $R = 1.41847181$  bohr). Furthermore, the minimum energy for  $\nu = 0.37039$  gives an energy  $E = -1.1744840$  au; that is, we have obtained the energy of the experimentally observed ground state of molecular hydrogen with a precision of  $1 \times 10^{-5}$  and a corresponding error in bond length of just 1.24%. This last result must be compared with the difference calculated by Aringazin and Kucherenko, 19.6%, to appreciate the importance of our finding.

Our approach to the hydrogen molecule, named from here onward as the Pérez-Marín-Riera approach to the restricted three-body Santilli-Shillady of the hydrogen molecule or M3CPM-R, encompasses more than the sole calculation of the minimum energy. With it, we can reproduce the whole set of data points of the KSM ground state curve in the  $R \in [0.8, 3.2]$  interval.

### 3.2 Comparison of our data with KSM curve

As we have just mentioned, our approach to the isoelectronic movement provides an effective way to represent the ground state of  $H_2$ . Using the box shape and effective mass parameters found for the closest value to the exact energy of the ground state minimum, we have calculated the energy for several values of the distance between protons ranging from 0.4 to 6.0 bohr. The values obtained in this manner show a very significant behavior, a least in a defined interval  $R \in [0.8, 3.2]$ . We reproduce the values that Kolos and his collaborators obtained with a highly sophisticated computing method, shown with ours in Table 4 for comparison. As can be seen while reviewing the last column in the table, a difference appears in the fourth significant digit for the worst result and up to the fifth digit for the best, which is located at  $R = 1.40$  bohr.

Figure 3 illustrates the values for the energy as a function of  $R$  found by Kolos (big points) together with the curve (line) representing our data. Both data sets are identical to

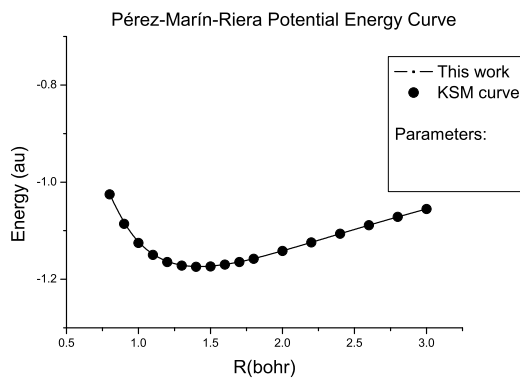


Fig. 3: Comparison between Kolos data and our exact restricted three-body model for the Hydrogen molecule (parameters are:  $\nu$  - mass;  $\xi_0$  - spheroidal shape).

each other up to the 4th significant digit; this is confirmed by a  $\chi^2$  statistical test ( $\chi^2 = 1.3522$  with  $gl = 17$ ), with a confidence level of 0.9999998. We state that by confining the isoelectronium, it is possible to reproduce the standard curve with a minimum computational calculation effort.

Again, if compare this result with that of the Aringazin-Kucherenko curve ( $\chi^2 = 410.239$  with  $gl = 17$ ), we state that the Aringazin curve differs completely from the KSM curve, as it was shown in Figure 2.

Both findings, up to six digit precision in minimum energy coincidence and whole curve reproduction, give support to our approach to the three-body Santilli-Shillady model. We can establish that the hypothesis on the isoelectronium movement is correct; that is, the orbiting of isoelectronium around both nuclei limits itself to a spheroidal region of space. Another way to express this behavior is that the formation of isoelectronium could be favored by the confinement of the molecule without changing its general properties.

The isoelectronium movement in a bound state together with the charge distribution confirms the explanation given by iso-chemistry to the following question: Why has the hydrogen molecule only two atoms? In our view, as soon as the molecule forms (isoelectronium) it becomes a bound system thus limiting the possibility of another hydrogen atom to be part of the molecule. In fact, the Pauli principle requires that the two valence electrons are correlated-bounded in a singlet state; as a result, the isoelectronium has spin zero. Consequently, no third electron can be bound via a conventional valence (see [3c] for details).

#### 4 Conclusions

The value for the minimum energy of the ground state of the hydrogen molecule has been obtained using the three-body Santilli-Shillady model. Other parameters involved, such as the optimum bond length or energies for several distances between nuclei, can not be verified with it. We have shown that after modifying the model, by introducing a condition on

$R^a)$	$\alpha^b)$	M3CP-M $c)$	KSM $d)$	Diff. $e)$
0.80	0.4188965	-1.024900	-1.0200565	0.0048435
0.90	0.4585059	-1.085753	-1.0836432	0.0021098
1.00	0.4964746	-1.125001	-1.1245396	0.0004614
1.10	0.5331055	-1.149680	-1.1500574	0.0003774
1.20	0.5686328	-1.164305	-1.1649352	0.0006302
1.30	0.6032813	-1.171876	-1.1723471	0.0004711
1.40	0.6371875	-1.174438	-1.1744757	0.0000377 $f)$
1.50	0.6705273	-1.173416	-1.1728550	0.0005610
1.60	0.7033789	-1.169826	-1.1685833	0.0012427
1.70	0.7358594	-1.164397	-1.1624586	0.0019384
1.80	0.7680469	-1.157664	-1.1550686	0.0025954
2.00	0.8319141	-1.141767	-1.1381329	0.0036341
2.20	0.8953906	-1.124237	-1.1201321	0.0041049
2.40	0.9589063	-1.106267	-1.1024226	0.0038444
2.60	1.0228130	-1.088534	-1.0857913	0.0027427
2.80	1.0871880	-1.071422	-1.0706831	0.0007389
3.00	1.1521880	-1.055136	-1.0573262	0.0021902
3.20	1.2179690	-1.039776	-1.0457995	0.0060235

Notes:  $a)$  Bond length (in bohr)  
 $b)$  Non linear variational parameter  
 $c)$  Our data in the present work with  $\xi_0 = 48.467148$  and  $\nu = 0.37039$   
 $d)$  Kolos, Szalewicz and Monhorst data from 1986 [6]  
 $e)$  Absolute value of the difference.  
 $f)$  Best approximation up to 6th significant digit

Table 4: Energies for the M3CP-M model and KSM curve

the isoelectronium orbit, it is possible to calculate a minimum energy for the ground state coincident with the experimental values up to the sixth significant digit. Furthermore, the modified three-body model of the hydrogen molecule, a confined three-body system, enables the reproduction of the whole curve of ground state energy in the range [0.80, 3.20] for the bond length. The physical interpretation to the confined isoelectronium model comprehends the isoelectronium itself, since the interaction between electrons while the quasi-particle is forming, implies its movement to be restricted to a defined region of space. The Santilli-Shillady orbits, the oo-shaped orbits, go beyond a way of speaking, they are a condition for the movement of the electron pair. This limitation in movement could be present in other states of electron pairs, such as the Cooper pairs of superconductivity, mainly in high Tc Superconductivity, for example.

The M3CP-M-R model of the hydrogen molecule introduced here represents an appropriate approach to study this molecule and gives support to the isoelectronium model introduced by Santilli and Shillady.

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