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On Possible Formation of Matter-Antimatter Exotic Molecular Structures

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Abstract

Possible formation of exotic matter-antimatter molecular structure is considered as one of the most challenging problems at International Laboratories of Particle Physics. In the present work, elaborate computer codes built for investigating four-body systems are employed for calculating the binding energies of exotic molecules composed of electrons, protons, muons, pions and their antiparticles. The results confirm the stability of these molecules against dissociation to their lowest possible channels. Based on these results, it is argued that possible creation of two universes immediately after the Big Bang should be considered. Particularly, it is proposed that an overlapping area might exist between the universe and antiuniverse in which continuous creation and annihilation of simple and complicated particle-antiparticle structures might occur. Antiparticles escaping from this area are considered as the origin of the minimal traces of antiparticles appearing in our universe. Recent interpretations of cosmic-rays and gamma-radiations observed at the edge of our universe could be thought of as evidences for supporting this argument. Furthermore, it is argued that possible formation of matter-antimatter molecular structures could open the gate in front of a new field of chemistry to be referred to as Antimatter Chemistry.

Subject Areas

Classical Physics

Keywords

Big Bang Theory, Universe and Antiuniverse, Four-Body Systems, Positroniums, Protoniums, Muoniums, Pioniums

1. Introduction

The existence of antiparticles was predicted by Paul Dirac [1] [2] and confirmed

through the pioneering discovery of anti-electrons (positrons) by Carl Anderson [3] in the thirties of the twentieth century. The fundamental property of particle-antiparticle pairs as stated by Dirac is that it collapses to electromagnetic radiation the moment they get closer to each other (see e.g. [4] [5]). Emilio Segerè and Owen Chamberlain's group [6] [7] [8] provided in 1955 a significant contribution in this field by discovering the antiproton in the Bevatron Laboratory built at the University of California Berkley. Further development of high energetic beams of protons at CERN and Fermilab indicated that electromagnetic radiations may lead to the production of a large number of particles and antiparticles on the top of which was the discovery of muon pairs (μ^+ and μ^-) [9] [10] and pion pairs (π^- π^+) as well as the neutral pion (π). Recent experiments [11] [12] [13] have confirmed the fact that the masses and spins of a proton and its antiproton are identical. This fact raised the question about the origin of our universe. Consequently, the "Big Bang" theory [14] [15] was proposed and successfully confirmed experimentally. Following this theory, an explosion occurring 13.7 billion years ago and lasting for 10^{-32} second led to the birth of a flood of identical amounts of particles and antiparticles [16]. The fact that almost negligible number of antiparticles exist in our universe is commonly attributed to symmetry breaking processes associated with the Big Bang [17]. These processes were followed by continuous particle-antiparticle annihilations, the leftover of which is our present universe. Other quite controversial theories were proposed by several authors (see e.g. [18] [19]), suggesting that matter and antimatter were confined in one and only one universe. The development of the string [20] and superstring [21] theories opened the floor in front of the development of multiverse theories (see [22] [23] [24] [25] [26]). Recently, an utmost interesting scenario was proposed [27] [28] [29] [30] that originally a collision between two branes took place. The kinetic energy of this collision was converted to particles, antiparticles and electromagnetic radiation. The particles were confined in our universe, whilst the recoiled hidden brane contains the antiuniverse. Both numbers of particles and antiparticles are identical.

On the other hand, other experimental facts about matter and antimatter are discussed in the literature. Martin Deutsch [31] was the first to show that an electron and an antielectron pairs could form quasi bound states (referred to as positroniums, Ps), with lifetimes ranging from 10^{-10} to 10^{-7} seconds. In 1995, a group working in ATHENA project at CERN [32] [33] [34] was able to create the first antiatom composed of an antielectron and antiproton in Laboratory (referred to as Antihydrogen). Scientists working at the ATRAP experiment [35] were able to increase the number of trapped Antihydrogens in the preceding few years.

Another revolutionary experiment led to the synthesizing of antiheliums (with nuclei composed of two antiprotons and two antineutrons [36]). Nevertheless, protoniums [37], true muoniums [38] and pioniums [39] were synthesized at CERN; a matter which supports the argument that matter, and antimatter could assume different channels during their interactions rather than annihilation

ones.

On the other hand, the possible formation of exotic molecular structures composed of matter and antimatter was proposed within the framework of the theory of four-body systems [40] [41] [42]. Formation of an exotic molecule composed of two positroniums, (the positronium molecule, Ps_2), was confirmed numerically by different authors (see e.g. Abel-Raouf [43] [44]) and experimentally by Mils' group [45]. Moreover, numerical evidences for the possible formation of different four-body systems with arbitrary mass ratios were established by Abdel-Raouf [46]. Our objectives in the present paper are threefold (see also [47]): 1) to give a brief account on the theory of four-body systems and show that their stability against dissociation to the lowest possible thresholds is incorporated in the theory; 2) to investigate the possible formation of exotic molecules composed of positroniums, protoniums, muoniums, pioniums, etc. using elaborate variational methods; and 3) to discuss the implications of synthesizing antiatoms and formation of Exotic Molecules on the coexistence of the universe and antiuniverse.

The next three sections are devoted to our three objectives. A complete list of the references mentioned in the text is given at the end of the paper.

2. The Four-Body Theory

Let m_1^-, m_2^+, m_a^-, and m_b^+ be four charged particle (say the first and third are particles, while the other two are antiparticles), with internal distances as illustrated in Figure 1.

The total Hamiltonian of such a four-body system has the form

$$H = -\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_a}\nabla_a^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 - \frac{\hbar^2}{2m_b}\nabla_b^2 + Z^2e^2\left(\frac{1}{r_{1a}} + \frac{1}{r_{2b}} - \frac{1}{r_{12}} - \frac{1}{r_{1b}} - \frac{1}{r_{2a}} - \frac{1}{r_{ab}}\right) \quad (1)$$

At any moment, different quasi atomic (two-body) and ionic (three + one) clusters are possible. Let us assume that (m_1^-, m_2^+) and (m_a^-, m_b^+) are two possible dissociating clusters with binding energies

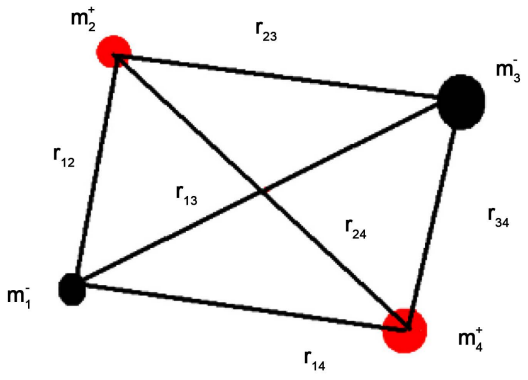

Figure 1. Relative coordinates of the four-body system.

$$E_{ab} = -\mu_{ab}\frac{Z^2e^2}{2\hbar^2} \quad \text{and} \quad E_{12} = -\mu_{12}\frac{Z^2e^2}{2\hbar^2}, \tag{2}$$

where

$$\mu_{ab} = \frac{m_a m_b}{m_a + m_b} \quad \text{and} \quad \mu_{12} = \frac{m_1 m_2}{m_1 + m_2} \tag{3}$$

are the reduced masses, respectively. The following two cases could be distinguished

$$\text{Case I:} \quad m_1 = m_a = m \quad \text{and} \quad m_2 = m_b = M \quad \text{where} \quad m \ll M \tag{4}$$

$$\text{Case II:} \quad m_1 = m_2 = m \quad \text{and} \quad m_a = m_b = M \quad \text{where} \quad m \ll M \tag{5}$$

Case I corresponds to the dissociation to an atom and an antiatom each is composed of a light and a heavy particle. The second case yields two separate tiny and heavy particle-antiparticle quasi atoms, the constituents of each of which are orbiting one another. It is obvious that case II assigns the lowest dissociation threshold. The dissociation to an ion (composed of three bodies) and a particle (or antiparticle) is also possible. However, the ion-particle binding energy is higher than case II. To absolutely guarantee that the four-body system is bound, it must have a total energy lower than the sum of the binding energies of all possible dissociation channels. (Remember that in case I, $\mu_{12} = \mu_{ab} = m$, and $E_{12} = E_{ab} = -mZ^4e^4/(2\hbar^2)$, whilst in case II $\mu_{12} = m/2$, $\mu_{ab} = M/2$, $E_{12} = -(m/2)Z^4e^4/(2\hbar^2)$ and $E_{ab} = -(M/2)Z^4e^4/(2\hbar^2)$. Remember also that $m = m_{e^-} = 1$ and $e^2 = 1$ mean that energies are measured in Hartree atomic units, whilst $m = m_{e^-} = 1/2$ and $e^2 = 2$ indicate that energies are measured in Rydberg).

Let us now define the binding energy $W(\sigma)$ by

$$W(\sigma) = E(\sigma) - (E_{12} + E_{ab}) \tag{6}$$

Clearly, the system is bound if and only if

$$W(\sigma) \le 0, \tag{7}$$

i.e. if the total energy $E(\sigma)$ is located lower than the sum of the binding energies of the dissociated clusters in the negative energy domain of the total Hamiltonian H. We refer to this sum as $E_{threshold}$ (or E_{thr}), where $E_{thr}(\mathrm{I}) = -2mZ^4e^4/(2\hbar^2)$ and $E_{thr}(\mathrm{II}) = -\frac{1}{2}(m+M)Z^4e^4/(2\hbar^2)$. Dividing (6) by E_{thr} leaves us with

$$\omega(\sigma) = \varepsilon(\sigma) - 1, \tag{8a}$$

where

$$\varepsilon(\sigma) = \frac{E(\sigma)}{E_{thr}} \quad \text{and} \quad \omega(\sigma) = \frac{W(\sigma)}{E_{thr}} \quad \text{with} \quad E_{thr} = E_{12} + E_{ab} \tag{8b}$$

Clearly, $E(\sigma)$ is related to $\omega(\sigma)$ by

$$E(\sigma) = (1 + \omega(\sigma))E_{thr}, \tag{8c}$$

Thus,

$$\omega(\sigma) \ge 0, \tag{9}$$

is a sufficient condition for the existence of the four-body system. Which is guaranteed if Equation (7) is fulfilled. Since, the potential energy part of H does not depend on the masses, therefore, the total Hamiltonian can be written as

$$\begin{aligned} H = &-\frac{\hbar^2}{2mM}\left[M\left(\nabla_1^2+\nabla_a^2\right)+m\left(\nabla_2^2+\nabla_b^2\right)\right] \\ &+Z^2e^2\left(\frac{1}{r_{12}}+\frac{1}{r_{ab}}-\frac{1}{r_{1a}}-\frac{1}{r_{2a}}-\frac{1}{r_{1b}}-\frac{1}{r_{2b}}\right). \end{aligned} \tag{10}$$

It is understood here that the indices 1, 2, a and b are dummy. Defining the mass ratio

$$\sigma = m/M \tag{11a}$$

and the reduced mass μ

$$\frac{1}{\mu}=\frac{1}{m}+\frac{1}{M}=\frac{M+m}{mM}=\frac{1+\sigma}{m}, \tag{11b}$$

the Hamiltonian takes the form

$$\begin{aligned} H = &-\frac{\hbar^2}{2\mu(M+m)}\left[M\left(\nabla_1^2+\nabla_a^2\right)+m\left(\nabla_2^2+\nabla_b^2\right)\right] \\ &+Z^2e^2\left(\frac{1}{r_{12}}+\frac{1}{r_{ab}}-\frac{1}{r_{1a}}-\frac{1}{r_{2a}}-\frac{1}{r_{1b}}-\frac{1}{r_{2b}}\right) \end{aligned} \tag{12}$$

$$\begin{aligned} = &-\frac{\hbar^2}{2\mu}\left[\frac{1}{1+\sigma}\left(\nabla_1^2+\nabla_a^2\right)+\frac{\sigma}{1+\sigma}\left(\nabla_2^2+\nabla_b^2\right)\right] \\ &+Z^2e^2\left(\frac{1}{r_{12}}+\frac{1}{r_{ab}}-\frac{1}{r_{1a}}-\frac{1}{r_{2a}}-\frac{1}{r_{1b}}-\frac{1}{r_{2b}}\right). \end{aligned} \tag{13}$$

Now, let us define the units of energy and length, respectively, as

$$\frac{\mu Z^4e^4}{2\hbar^2} \quad \text{is the unit of energy} \tag{14a}$$

$$\frac{\hbar^2}{\mu Z^2e^2} \quad \text{is the unit of length} \tag{14b}$$

Multiply the Hamiltonian by the reciprocal of the energy unit leaves us with

$$\begin{aligned} H = &-\frac{\hbar^2}{2\mu}\frac{2\hbar^2}{\mu Z^4e^4}\left[\frac{1}{1+\sigma}\left(\nabla_1^2+\nabla_a^2\right)+\frac{\sigma}{1+\sigma}\left(\nabla_2^2+\nabla_b^2\right)\right] \\ &+Z^2e^2\frac{2\hbar^2}{\mu Z^4e^4}\left(\frac{1}{r_{12}}+\frac{1}{r_{ab}}-\frac{1}{r_{1a}}-\frac{1}{r_{2a}}-\frac{1}{r_{1b}}-\frac{1}{r_{2b}}\right) \end{aligned}$$

$$\begin{aligned} = &-\left(\frac{\hbar^2}{\mu Z^2e^2}\right)^2\left[\frac{1}{1+\sigma}\left(\nabla_1^2+\nabla_a^2\right)+\frac{\sigma}{1+\sigma}\left(\nabla_2^2+\nabla_b^2\right)\right] \\ &+2\left(\frac{\hbar^2}{\mu Z^2e^2}\right)\left(\frac{1}{r_{12}}+\frac{1}{r_{ab}}-\frac{1}{r_{1a}}-\frac{1}{r_{2a}}-\frac{1}{r_{1b}}-\frac{1}{r_{2b}}\right). \end{aligned} \tag{15}$$

Since we took $\frac{\hbar^2}{\mu Z^2e^2}$ to be equal to unity, then the Hamiltonian could final-

ly be given by:

$$H=\left\{\frac{-1}{1+\sigma}\left[\nabla_1^2+\nabla_a^2+\sigma\left(\nabla_2^2+\nabla_b^2\right)\right]\right\}_T+\left\{\frac{2}{r_{12}}+\frac{2}{r_{ab}}-\frac{2}{r_{1a}}-\frac{2}{r_{2a}}-\frac{2}{r_{1b}}-\frac{2}{r_{2b}}\right\}_V, \quad (16)$$

where T and V assign, respectively, the total kinetic and potential energy operators of the system.

It is important from now on to indicate that the units of energy and length defined at (14a, 14b) are independent of the choices mentioned at Equations (4) and (5), *i.e.* independent of the subclusters, or dissociation channels, of the molecule. The same argument is also valid for the Hamiltonian (16).

Now, if $\{|\psi_k\rangle\}$ is the set of exact wavefunctions of the four-body system, such that:

$$\psi_k=\psi_k(r_1,r_2,\cdots), \quad (17)$$

and

$$\langle\Psi_{k'}|\Psi_{k'}\rangle=\int\Psi_k^*\Psi_{k'}\mathrm{d}\tau=\delta_{kk'}, \quad (18)$$

where $\mathrm{d}\tau$ is the volume element, therefore, the bound-states of the system are identical with the negative spectrum of the Hamiltonian within the space $\{|\psi_k\rangle\}$, *i.e.*, they are the eigenvalues of the Schrödinger equation

$$H|\psi_k\rangle=E_k|\psi_k\rangle, \quad (19)$$

and can be determined by,

$$E_k=\langle\psi_k|H|\psi_k\rangle, \quad (20)$$

such that

$$E_k\le E_{k+1},\ \text{for all } k\ge 1. \quad (21)$$

Obviously, if $E_k\ge 0$ for all k's, then the total Hamiltonian H does not possess any negative spectrum and the quantum mechanical system cannot form a bound-state, in other words, the molecule consisting of the four bodies (m_1^-, m_2^+, m_a^-, and m_b^+) simply cannot exist.

2.1. The Rayleigh-Ritz' Variational Method

Since H is a four-body Hamiltonian, the non-separability of V ceases the possibility of obtaining any exact solution for Equation (19), and we are obliged to choose between different approximations. The most mathematically reliable one is the conventional Rayleigh-Ritz' variational method [48]. It is the first variational method of bound state type which has been employed in the treatment of the ground states of atomic, molecular and nuclear systems. It was also extended by Hylleraas-Undheim (see [48]) to the treatment of the excited states of any quantum mechanical system.

The method can be displayed as follows: consider the non-relativistic time independent quantum mechanical system defined in the preceding section, The Schrödinger's equation is equivalent in form to the conventional eigenvalue problem:

$$H|\psi\rangle = E|\psi\rangle, \tag{22}$$

or

$$(H-E)|\psi\rangle = 0, \tag{23}$$

where E and H are the total energy and Hamiltonian, respectively, of a quantum mechanical system described by the vector $|\psi\rangle$. The Schrödinger constraint can be stated according to Equation (23) as follows: a true physical system or process described by the observable ($H-E$) is well expressed, microscopically, by the expansion space $|\psi\rangle$ if and only if Schrödinger vector $(H-E)|\psi\rangle$ defines a null space. Also, Equation (23) fulfills the variational principle:

$$\partial\langle\psi|H-E|\psi\rangle = 0 \tag{24}$$

and possesses the eigenvalues:

$$E_k = \langle\psi_k|H|\psi_k\rangle/\langle\psi_k|\psi_k\rangle \tag{25}$$

Equations (23), (24) and (25) imply a one-to-one correspondence between the E_k's and $|\psi_k\rangle$'s once the degeneracy has been removed. Consequently, one can order the E_k's such that

$$E_k \le E_{k+1}, \quad \text{for } k = 1,2,\cdots, \tag{26}$$

where E_1 is the first (lowest) eigenvalue.

Now, the verification of Schrödinger's constraint requires the exact knowledge of the terms E, H and $|\psi\rangle$. In practice, however, $|\psi\rangle$ is always unknown and the parameter E is not given for the boundary value problems. For this, there was a necessity of using approximate methods to get a solution for physical problems.

In Rayleigh-Ritz variational method a trial expansion space $|\psi_t^{(n)}\rangle$ is selected which defines a hypothetical physical system such that

$$\psi_t^{(n)} = \sum_k^n a_k|\psi_{tk}\rangle \tag{27}$$

where n is the dimension of $|\psi_{tk}^{(n)}\rangle$, and

$$\langle\psi_{tk}^{(n)}|\psi_{tk'}^{(n)}\rangle = \delta_{kk'}, \quad \text{for } k,k' = 1,2,\cdots,n \tag{28}$$

where $\delta_{kk'}$ is the Kroneker-delta. Equation (28) will then reduce to

$$\partial\langle\psi_t^{(n)}|H-E|\psi_t^{(n)}\rangle = 0 \tag{29}$$

All $|\psi_{tk}^{(n)}\rangle$'s are, due to Rayleigh-Ritz variational method, generated from one basis set of vectors $\{|\chi_i\rangle\} \subset D_H$ where D_H is the H-domain, *i.e.*,

$$|\psi_{tk}^{(n)}\rangle = \sum_{i=1}^n c_{ik}|\chi_i\rangle \tag{30}$$

Consequently, Equation (29) can be written for each k as the system of secular equations:

$$\sum_{j=1}^n c_{jk}\left[\langle\chi_i|H|\chi_j\rangle - E_{nk}\langle\chi_i|\chi_j\rangle\right] = 0, \quad i = 1,2,\cdots,n \tag{31}$$

which is meaningful if and only if the determinant Δ_{nk} satisfies the relation

$$\Delta_{nk} = \det\left(H_{ij} - E_{nk}S_{ij}\right) = 0, \tag{32}$$

where

$$H_{ij} = \left\langle \chi_i \middle| H \middle| \chi_j \right\rangle, \tag{33a}$$

and

$$S_{ij} = \left\langle \chi_i \middle| \chi_j \right\rangle \tag{33b}$$

The eigenvalues obtained by (31) are ordered such that:

$$E_{n1} \le E_{n2} \le \cdots \le E_{nn}, \tag{34}$$

is satisfied.

Rayleigh and Ritz (see e.g. [34] [35]) proved the important relation between E_{n1} and the first exact energy level of the system E_1, namely that

$$E_1 \le E_{n1}, \quad \text{for } n > 0, \tag{35a}$$

i.e., for any choice of the components $\left|\psi_{tk}^{(n)}\right\rangle$, the first variational energy is an upper bound to the exact one. Hylleraas and Undheim (see e.g. [34]), moreover, have shown that if the condition (34) is fulfilled, we then get

$$E_k \le E_{nk}, \quad \text{for } k = 1,2,\cdots,n. \tag{35b}$$

McDonald (see also [48] and references therein), on the other hand, demonstrated that, if the trial expansion space is enlarged by exactly one component such that

$$\left\langle \psi_{tk}^{(n+1)} \middle| \psi_{tk'}^{(n+1)} \right\rangle = \delta_{kk'}, \quad \text{for } k,k' = 1,2,\cdots,n+1, \tag{36}$$

then the following successive relations are always valid:

$$E_{n+11} \le E_{n1} \le E_{n+12} \le \cdots \le E_{n+1n} \le E_{nn} \le E_{n+1n+1}, \tag{37a}$$

$$E_{n+1k} \le E_{n+1k'} \quad \text{for } k \le k', \tag{37b}$$

$$E_{n+1k+1} \le E_{nk'} \quad \text{for } k > k', \tag{37c}$$

$$E_k \le E_{n+1k} \le E_{nk} \le E_{n-1k} \le \cdots \le E_{1k}. \tag{37d}$$

Equations (37) imply that the existence of any negative E_{nk} ensures the existence of corresponding bound state of the four-body system, and for this reason we are led to say that Rayleigh-Ritz' variational method provides an approximate solution of (22).

2.2. Theoretical Proof of the Existence of Four-Body Molecules

The four-body theorem states that "If σ is the mass ratio characteristic to any particle-antiparticle pair, then the existence of two molecules with $\sigma = 0$ and $\sigma = 1$ is a sufficient condition for the existence of all molecules with σ lying between 0 and 1".

To prove this theorem, let us go back to Equations (6) and (8) and define the following quantities: $E_1(\sigma)$ is the ground-state energy of the whole system,

and $W(\sigma)$ is the binding energy with which the four-body system is stable against any possible dissociation. Thus, it is obvious that the molecule is bound if and only if $W(\sigma)$ satisfies the relation:

$$W(\sigma) = E_1(\sigma) - E_{thr} < 0. \tag{38}$$

Now, from (16) we have

$$\frac{\partial H}{\partial \sigma} = \frac{1}{(1+\sigma)^2}\left(\nabla_1^2 + \nabla_a^2 - \nabla_2^2 - \nabla_b^2\right) \tag{39}$$

and

$$\frac{\partial^2 H}{\partial \sigma^2} = -\frac{2}{1+\sigma}\frac{\partial H}{\partial \sigma} \tag{40}$$

Remember that H is the total Hamiltonian of the system without any restriction, but the one regarding the definition of the unit energy and unit length. On the other hand, Equation (8a) yields

$$\frac{\partial \omega}{\partial \sigma} = \frac{\partial \varepsilon}{\partial \sigma} \text{ and } \frac{\partial^2 \omega}{\partial \sigma^2} = \frac{\partial^2 \varepsilon}{\partial \sigma^2}. \tag{41a}$$

While Equations (6) and (8b) imply

$$\frac{\partial W}{\partial \sigma} = \frac{\partial E}{\partial \sigma} \text{ and } \frac{\partial^2 W}{\partial \sigma^2} = \frac{\partial^2 E}{\partial \sigma^2}. \tag{41b}$$

Now, let us restrict ourselves to the ground state of the four-body system and assume that $E_1(\sigma)$ and $|\psi_1\rangle$ are, respectively, the corresponding exact ground state energy and wavefunction. Therefore, they satisfy the relations:

$$H|\psi_1\rangle = E_1|\psi_1\rangle \text{ or } (H - E_1)|\psi_1\rangle = 0, \tag{42}$$

which imply

$$\frac{\partial(H - E_1)}{\partial \sigma}|\psi_1\rangle = -(H - E_1)\left|\frac{\partial \psi_1}{\partial \sigma}\right\rangle \tag{43}$$

and

$$\langle\psi_1|\frac{\partial(H - E_1)}{\partial \sigma}|\psi_1\rangle = -\langle\psi_1|(H - E_1)\left|\frac{\partial \psi_1}{\partial \sigma}\right\rangle \tag{44}$$

Since H is Hermitian, the right-hand side of (44) is zero, and we have;

$$\frac{\partial E_1}{\partial \sigma} = \langle\psi_1|\frac{\partial H}{\partial \sigma}|\psi_1\rangle = \frac{1}{(1+\sigma)^2}\langle\psi_1|\nabla_1^2 + \nabla_a^2 - \nabla_2^2 - \nabla_b^2|\psi_1\rangle \tag{45}$$

Defining the expectation values for the kinetic energy operators T_a and T_b as

$$\begin{aligned} \langle T_a\rangle &= \langle\psi_1|\frac{-1}{1+\sigma}\left(\nabla_1^2 + \nabla_a^2\right)|\psi_1\rangle \\ \langle T_b\rangle &= \langle\psi_1|\frac{-1}{1+\sigma}\left(\nabla_2^2 + \nabla_b^2\right)|\psi_1\rangle. \end{aligned} \tag{46}$$

Equations (45) can then be written as:

$$\frac{\partial E_1}{\partial \sigma} = \frac{1}{1+\sigma}\left(\frac{\langle T_b\rangle}{\sigma} - \langle T_a\rangle\right). \tag{47}$$

Since $|\psi_1\rangle$ is symmetric with respect to the coordinates of the two particles a and b, we expect that $\langle T_a\rangle$ equals $\langle T_b\rangle$ at $\sigma=1$, so that

$$\left.\frac{\partial E_1}{\partial\sigma}\right|_{\sigma=1}=0. \tag{48}$$

Using (41b), we get

$$\left.\frac{\partial W_1}{\partial\sigma}\right|_{\sigma=1}=0. \tag{49}$$

Now, operate with $\left\langle\frac{\partial\psi_1}{\partial\sigma}\right|$ on (43) from the left, we get:

$$\left\langle\frac{\partial\psi_1}{\partial\sigma}\middle|\frac{\partial(H-E_1)}{\partial\sigma}|\psi_1\right\rangle=-\left\langle\frac{\partial\psi_1}{\partial\sigma}\middle|(H-E_1)\middle|\frac{\partial\psi_1}{\partial\sigma}\right\rangle \tag{50}$$

The variational theory demands that (50)

$$\left\langle\frac{\partial\psi_1}{\partial\sigma}\middle|(H-E_1)\middle|\frac{\partial\psi_1}{\partial\sigma}\right\rangle\geq 0. \tag{51}$$

Therefore (50) leads to

$$-\left\langle\frac{\partial\psi_1}{\partial\sigma}\middle|\frac{\partial(H-E_1)}{\partial\sigma}|\psi_1\right\rangle\geq 0. \tag{52}$$

On the other hand, Equation (43) provides us with

$$\frac{\partial}{\partial\sigma}\left[\frac{\partial(H-E_1)}{\partial\sigma}|\psi_1\right\rangle\Big]=-\frac{\partial}{\partial\sigma}\left[\frac{\partial(H-E_1)}{\partial\sigma}\middle|\frac{\partial\psi_1}{\partial\sigma}\right\rangle\Big]. \tag{53}$$

$$\therefore\frac{\partial^2(H-E_1)}{\partial\sigma^2}|\psi_1\rangle+\frac{\partial(H-E_1)}{\partial\sigma}\left|\frac{\partial\psi_1}{\partial\sigma}\right\rangle=-\frac{\partial(H-E_1)}{\partial\sigma}\left|\frac{\partial\psi_1}{\partial\sigma}\right\rangle-(H-E_1)\left|\frac{\partial^2\psi_1}{\partial\sigma^2}\right\rangle$$

or

$$\frac{\partial^2(H-E_1)}{\partial\sigma^2}|\psi_1\rangle+2\frac{\partial(H-E_1)}{\partial\sigma}\left|\frac{\partial\psi_1}{\partial\sigma}\right\rangle+(H-E_1)\left|\frac{\partial^2\psi_1}{\partial\sigma^2}\right\rangle=0 \tag{54}$$

Operating on this equation by $\langle\psi_1|$ from the left, we obtain

$$\langle\psi_1|\frac{\partial^2(H-E_1)}{\partial\sigma^2}|\psi_1\rangle+2\langle\psi_1|\frac{\partial(H-E_1)}{\partial\sigma}\left|\frac{\partial\psi_1}{\partial\sigma}\right\rangle+\langle\psi_1|(H-E_1)\left|\frac{\partial^2\psi_1}{\partial\sigma^2}\right\rangle=0. \tag{55}$$

Again, the Hermeticity of H yields

$$\langle\psi_1|(H-E_1)\left|\frac{\partial^2\psi_1}{\partial\sigma^2}\right\rangle=0, \tag{56}$$

so that

$$\langle\psi_1|\frac{\partial^2(H-E_1)}{\partial\sigma^2}|\psi_1\rangle=-2\langle\psi_1|\frac{\partial(H-E_1)}{\partial\sigma}\left|\frac{\partial\psi_1}{\partial\sigma}\right\rangle$$

using (52) we get

$$\langle\psi_1|\frac{\partial^2(H-E_1)}{\partial\sigma^2}|\psi_1\rangle\geq 0$$

so that

$$\frac{\partial^2 E_1}{\partial \sigma^2} \le \langle \psi_1 | \frac{\partial^2 H}{\partial \sigma^2} | \psi_1 \rangle , \tag{57}$$

substituting from (45) into (57), we find

$$\frac{\partial^2 E_1}{\partial \sigma^2} \le -\frac{2}{1+\sigma} \langle \psi_1 | \frac{\partial H}{\partial \sigma} | \psi_1 \rangle , \tag{58}$$

using (45)

$$\frac{\partial^2 E_1}{\partial \sigma^2} \le -\frac{2}{1+\sigma} \frac{\partial E_1}{\partial \sigma} , \tag{59}$$

and using (41a, 41b)

$$\frac{\partial^2 W_1}{\partial \sigma^2} \le -\frac{2}{1+\sigma} \frac{\partial W_1}{\partial \sigma} , \tag{60}$$

Now, Equation (47) states that $\frac{\partial E_1}{\partial \sigma}$, and consequently $\frac{\partial E_1}{\partial \sigma}$, is a continuous function of σ in the interval (0, 1). This continuity together with the boundary condition (49) and the inequality (60) demand

$$\frac{\partial W_1}{\partial \sigma} \ge 0 \quad \text{for all } \sigma \in (0,1) , \tag{61}$$

that is to say $W_1(\sigma)$ is a monotonic function of σ in this interval. Also (60) and (61) lead to the inequality:

$$\frac{\partial^2 W_1}{\partial \sigma^2} \le 0 \quad \text{for all } \sigma \in (0,1) . \tag{62}$$

Thus $W_1(\sigma)$ is a concave function with the characteristics

$$W_1(0) \le W_1(\sigma) \le W_1(1) \quad \text{for all } \sigma \in (0,1) \tag{63}$$

and it is bound within the triangle $(0, W_1(0)), (0, W_1(1)), (1, W_1(1))$, see **Figure 2**.

The inequality (63) states that: if $W_1(0)$ and $W_1(1)$ are negative, then $W_1(\sigma)$ will be negative at all $\sigma \in (0,1)$. That is to say if the four-body system has a ground state at $\sigma = 0$, which corresponds in case I with $Z = 1$, to the adiabatic treatment of H_2 molecule, and at $\sigma = 1$, corresponds, at the same condition, to the positronium molecule Ps_2 that is a bound state composed of

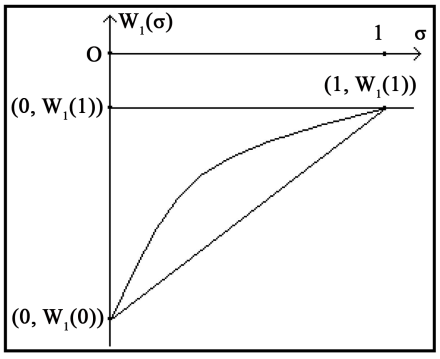

Figure 2. Behavior of $W_1(\sigma)$ with the variation of σ.

two electrons and two positrons, it has a ground state at all $\sigma \in (0,1)$. In fact, it has been shown [28] [29] [30] that, starting from the inequality (56), the existence of a four-body system with $\sigma = 1$ is a sufficient condition for the existence of any molecule with $0 \le \sigma \le 1$, so that the existence of a positronium molecule for example implies the existence of molecule composed of a hydrogen and antihydrogen. Further, more the following points have been concluded:

1) If the four-body system defined by the Hamiltonian (16), exists at $\sigma = 0$ and $\sigma = 1$, then all molecules with σ lying between 0 and ∞ should exist.

2) If $W_k = E_k - 2E_{ab}^k$, where E_k^{ab} is the k^{th} state of the pair m_a^-, m_b^+, the following two conclusions are true:

a) If the k^{th} state of $m_1^- m_2^+ m_3^- m_4^+$ exists at $\sigma = 0$ and $\sigma = 1$, the k-th state of $m_1^- m_2^+ m_3^- m_4^+$ exists at all $0 \le \sigma \le 1$.

b) $W_k(0) \le W_k(\sigma) \le W_k(1)$ (64)

The above theorem and conclusions suggest that systems like $e^- \pi^+ \pi^- e^+$, $e^- \mu^+ \mu^- e^+, \mu^- \pi^+ \pi^- \mu^+, \cdots$ etc. may also exist as molecular structures.

On the other hand, the preceding theorem has been extended [30] to the cases at which M is replaced by nM, where $n > 1$, which predicts the existence of systems like antihydrogen-deuterium ($\bar{H}D$) and antihydrogen-tritium ($\bar{H}T$) as bound states. Figure 3 shows a general schematic diagram for systems with M is replaced by nM where $n > 1$.

For these systems, the Hamiltonian (1) is replaced by:

$$H = -\frac{\hbar^2}{2m_e}\left(\nabla_1^2 + \nabla_a^2\right) - \frac{\hbar^2}{2M_p}\nabla_2^2 - \frac{\hbar^2}{2nM_p}\nabla_b^2 + Z^2 e^2\left(\frac{1}{r_{12}} + \frac{1}{r_{ab}} - \frac{1}{r_{1a}} - \frac{1}{r_{2a}} - \frac{1}{r_{1b}} - \frac{1}{r_{2b}}\right), \quad (65)$$

Also, Equation (16) takes the following form

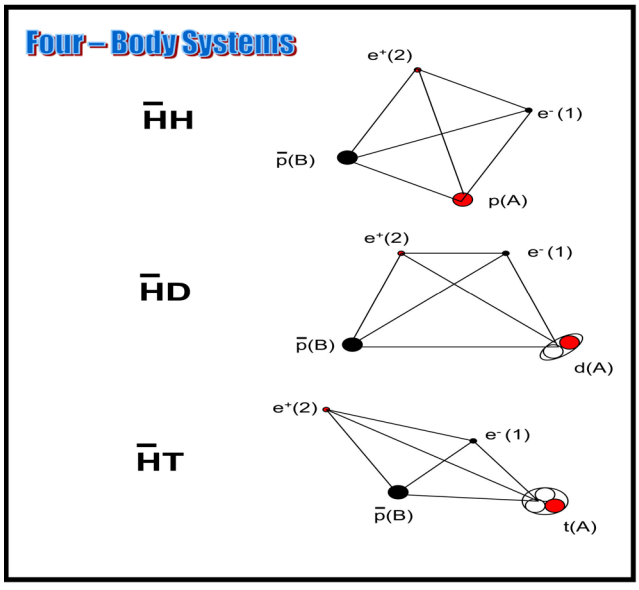

Figure 3. Various four-body systems.

$$H = \left\{ \frac{-1}{1+\sigma}\left[\nabla_1^2 + \nabla_a^2 + \sigma\left(\nabla_2^2 + \frac{1}{n}\nabla_b^2 \right) \right] \right\}_T + \left\{ \frac{2}{r_{12}} + \frac{2}{r_{ab}} - \frac{2}{r_{1a}} - \frac{2}{r_{2a}} - \frac{2}{r_{1b}} - \frac{2}{r_{2b}} \right\}_V, \tag{66}$$

where $n=2$ for $\bar{\mathrm{H}}\mathrm{D}$ and $n=3$ for $\bar{\mathrm{H}}\mathrm{T}$ molecules.

The binding energy $W_1(\sigma)$ for such molecules will be given by:

$$W_1(\sigma) = E_1(\sigma) - E_{thr} - \Delta \tag{67}$$

where

$$\Delta = \frac{(n-1)\sigma}{2(n\sigma+1)} \tag{68}$$

It is clear that Δ is always positive definite, so if $W_1(\sigma)$ is negative for $n=1$, it is necessarily negative for all $n>1$. This means that if the four-body molecule $m_1^- m_2^+ m_3^- m_4^+$ exists at $n=1$ for a given σ, it exists at all values of n for the same σ. This in turn means that the existence of $\bar{\mathrm{H}}\mathrm{H}$ molecule implies the existence of $\bar{\mathrm{H}}\mathrm{D}$ and $\bar{\mathrm{H}}\mathrm{T}$ molecules. In particular, the following conclusions are valid:

1) If $W_k = E_k - E_k^{a2} - E_k^{1b}$ where E_k^{a2} and E_k^{1b} are both the *k*-th excited states of the clusters *a*-2 and 1-*b*, respectively, and E_k is the corresponding singlet excited state of the four-body system, the following statements are true:

a) If the *k*-th excited state of 12ab exists at $\sigma=1$, $n=1$, then the *k*-th excited state of 12ab exists also at $0\le\sigma\le 1$ for all $n\ge 1$.

b) $W_k(0)\le W_k(\sigma)\le W_k(1)$.

The proof of a) follows from the definition of W_k and the generalization of the theorem for $k>1$, while b) is a result of a) and is a generalization of (64).

2.3. The Virial Theorem

This theory predicts the upper bound energies E_k^v to the real bound state energies E_k by replacing the coordinates r_{ij} by αr_{ij} where α is a variational parameter. Since the kinetic energy operator is second order in $(\frac{\partial}{\partial r_{ij}})$ while the potential energy operator is first order of $(\frac{1}{r_{ij}})$, we may define the virial Hamiltonian as

$$H_v = \frac{1}{\alpha^2}T + \frac{1}{\alpha}V \tag{69}$$

and since the virial energy E_k is

$$E_k^v = \frac{\left\langle \psi_{tk}^{(n)} \middle| H \middle| \psi_{tk}^{(n)} \right\rangle}{\left\langle \psi_{tk}^{(n)} \middle| \psi_{tk}^{(n)} \right\rangle},$$

we have

$$E_k^v = \frac{\left\langle \psi_{tk}^{(n)} \middle| \frac{1}{\alpha^2} T + \frac{1}{\alpha} V \middle| \psi_{tk}^{(n)} \right\rangle}{\left\langle \psi_{tk}^{(n)} \middle| \psi_{tk}^{(n)} \right\rangle} = \frac{1}{\alpha^2} T_{ex} + \frac{1}{\alpha} V_{ex}, \tag{70}$$

where,

$$T_{ex} = \frac{\left\langle \psi_{tk}^{(n)} \middle| T \middle| \psi_{tk}^{(n)} \right\rangle}{\left\langle \psi_{tk}^{(n)} \middle| \psi_{tk}^{(n)} \right\rangle} \text{ and } V_{ex} = \frac{\left\langle \psi_{tk}^{(n)} \middle| V \middle| \psi_{tk}^{(n)} \right\rangle}{\left\langle \psi_{tk}^{(n)} \middle| \psi_{tk}^{(n)} \right\rangle} \tag{71}$$

Now, the upper bound states are obtained by minimization with respect to α. Doing so, Equation (70) gives:

$$\frac{\partial E_k^v}{\partial \alpha} = -\frac{2}{\alpha^3} T_{ex} - \frac{1}{\alpha^2} V_{ex} = 0, \tag{72}$$

and

$$\alpha = -\frac{2T_{ex}}{V_{ex}}. \tag{73}$$

Substituting from (74) into (71), we obtain

$$E_k^v = \frac{-V_{ex}^2}{4T_{ex} \left\langle \psi_{tk}^{(n)} \middle| \psi_{tk}^{(n)} \right\rangle} = \frac{-\left\langle \psi_{tk}^{(n)} \middle| V \middle| \psi_{tk}^{(n)} \right\rangle^2}{4\left\langle \psi_{tk}^{(n)} \middle| T \middle| \psi_{tk}^{(n)} \right\rangle \left\langle \psi_{tk}^{(n)} \middle| \psi_{tk}^{(n)} \right\rangle}, \tag{74}$$

this is known as the virial energy.

3. Numerical Treatment of Four-Body Systems

Although the theory and corollaries presented in the preceding section provide us with a rigorous proof for the possible formation of the four-body systems defined by the Hamiltonian (1), the values of their total energies as well as the forms of their wavefunctions remain undefined. The present section is devoted to the numerical investigation of these quantities within the framework of Rayleigh-Ritz variational method discussed in Section 2.2. The next two subsections are concerned with the representation of the operators and the wavefunctions adherent to the four-body systems.

3.1. Kinetic and Potential Energy Operators

Let us consider **Figure 1** and recall the Hamiltonian (16)

$$H = \left\{ \frac{-1}{1+\sigma} \left[\nabla_1^2 + \nabla_a^2 + \sigma \left(\nabla_2^2 + \nabla_b^2 \right) \right] \right\}_T + \left\{ \frac{2}{r_{12}} + \frac{2}{r_{ab}} - \frac{2}{r_{1a}} - \frac{2}{r_{2a}} - \frac{2}{r_{1b}} - \frac{2}{r_{2b}} \right\}_V,$$

which can be written as

$$H = \frac{-1}{1+\sigma} \left[T_1 + T_a + \sigma \left(T_2 + T_b \right) \right] + V \tag{75}$$

The kinetic energy operator contains terms of the form

$$T_i = -\nabla_i^2;\ i = 1, a, 2, b \tag{76}$$

In terms of the coordinate system given in Figure 1, the operator in (76) can be written as

$$\nabla_i^2 = \sum_{j\neq i, j<k} \left(\frac{\partial^2}{\partial r_{ij}^2} + \frac{2}{r_{ij}} \frac{\partial}{\partial r_{ij}} \right) + 2 \sum_{j\neq i} \sum_{k\neq i} \cos\theta_{ij,ik} \frac{\partial^2}{\partial r_{ij} \partial r_{ik}} \tag{77}$$

and

$$\cos\theta_{ij,ik} = \frac{r_{ij}^2 + r_{ik}^2 - r_{jk}^2}{2 r_{ij} r_{ik}} \tag{78}$$

3.2. Hylleraas' Coordinates

Our system must be described in a more suitable system of coordinates; this is because the components of the spherical polar coordinates r_{ij} are not orthogonal to each other and so highly dependent. Besides, the new system must take in consideration the correlation relation between different particles in the molecule. We notice that the interaction relation between different particles in our system is not one-to-one particle interaction; instead, it is one-to-two.

Let us replace the relative coordinates with a Hylleraas' coordinate system consisting of confocal ellipses and hyperbolas defined as

$$s_i = \left(r_{ia} + r_{ib}\right)/r_{ab};\quad i = 1, 2 \tag{79a}$$

$$t_i = \left(r_{ia} - r_{ib}\right)/r_{ab};\quad i = 1, 2 \tag{79b}$$

$$s_a = \left(r_{1a} + r_{2a}\right)/r_{12},\quad s_b = \left(r_{1b} + r_{2b}\right)/r_{12}, \tag{79c}$$

$$t_a = \left(r_{1a} - r_{2a}\right)/r_{12},\quad t_b = \left(r_{1b} - r_{2b}\right)/r_{12}, \tag{79d}$$

$$u = r_{12}/r_{ab},\quad v = r_{ab}. \tag{79e}$$

As it is evident s_i, s_a and s_b are constants on ellipses the distance between their two foci are r_{ab} for s_i and r_{12} for s_a and s_b, while t_i, t_a and t_b are constants on hyperbolas again the distances between their two foci are r_{ab} for t_i and r_{12} for t_a and t_b. It is clear that s goes from 1 to infinity, t goes from -1 to 1, and v goes from 0 to infinity. In addition to these variables there are also the angles of rotation Φ's about the axis joining the two foci.

The point now is to write the Hamiltonian of the system in terms of these coordinates. The partial derivatives with respect to r_{ia} and r_{ib} can be expressed in terms of s_i and t_i as follows:

$$\frac{\partial}{\partial r_{1a}} = \frac{\partial s_1}{\partial r_{1a}} \frac{\partial}{\partial s_1} + \frac{\partial t_1}{\partial r_{1a}} \frac{\partial}{\partial t_1} \tag{80}$$

then

$$\frac{\partial}{\partial r_{1a}} = \frac{1}{v}\left(\frac{\partial}{\partial s_1} + \frac{\partial}{\partial t_1} \right),\quad \frac{\partial^2}{\partial r_{1a}^2} = \frac{1}{v^2}\left(\frac{\partial^2}{\partial s_1^2} + 2\frac{\partial^2}{\partial s_1 \partial t_1} + \frac{\partial^2}{\partial t_1^2} \right), \tag{81a}$$

and so on. Finally, we have

$$\frac{\partial}{\partial r_{12}} = \frac{1}{v}\frac{\partial}{\partial u}, \quad \frac{\partial^2}{\partial r_{12}^2} = \frac{1}{v^2}\frac{\partial^2}{\partial u^2} \tag{81b}$$

We also have

$$\cos\theta_{ij,ik} = \frac{r_{ij}^2 + r_{ik}^2 - r_{jk}^2}{2r_{ij}r_{ik}}, \qquad i = 1,2$$

$$= \frac{\frac{v^2}{4}\left[\left(s_i + t_i\right)^2 + \left(s_i - t_i\right)^2\right] - v^2}{\frac{2v^2}{4}\left(s_i + t_i\right)\left(s_i - t_i\right)},$$

$$\therefore \cos\theta_{ia,ib} = \frac{s_i^2 + t_i^2 - 2}{s_i^2 - t_i^2}. \tag{82}$$

Now, the kinetic energy operator (for example) T_1 can be written as

$$\begin{aligned} T_1 = &-\frac{4}{v^2}\frac{1}{s_1^2 - t_1^2}\left[\left(s_1^2 - 1\right)\frac{\partial^2}{\partial s_1^2} + \left(1 - t_1^2\right)\frac{\partial^2}{\partial t_1^2} + 2s_1\frac{\partial}{\partial s_1} - 2t_1\frac{\partial}{\partial t_1}\right] \\ &-\frac{1}{v^2}\left[\frac{\partial}{\partial u} + \frac{2}{u} + 2\left(\cos\theta_{12,1a} + \cos\theta_{12,1b}\right)\frac{\partial}{\partial s_1}\right. \\ &\left. + 2\left(\cos\theta_{12,1a} - \cos\theta_{12,1b}\right)\frac{\partial}{\partial t_1}\right]\frac{\partial}{\partial u}, \end{aligned} \tag{83}$$

Similar forms can be derived for T_2, T_a and T_b.

On the other hand, the potential energy operator which is given by:

$$V = 2\left(\frac{1}{r_{12}} + \frac{1}{r_{ab}} - \frac{1}{r_{1a}} - \frac{1}{r_{2a}} - \frac{1}{r_{1b}} - \frac{1}{r_{2b}}\right),$$

will be modified to

$$V = \frac{2}{v}\left[\left(\frac{1}{u} + 1\right) - \frac{4s_1}{s_1^2 - t_1^2} - \frac{4s_2}{s_2^2 - t_2^2}\right] \tag{84}$$

3.3. The Volume Element of the System

Two forms for the volume element $\mathrm{d}\tau$ could be distinguished (see Equation (79)):

1) v is variable:

$$\mathrm{d}\tau = \frac{v^8}{64}\left(s_1^2 - t_1^2\right)\left(s_2^2 - t_2^2\right)\mathrm{d}s_1\mathrm{d}s_2\mathrm{d}t_1\mathrm{d}t_2\mathrm{d}v\sin\theta_v\mathrm{d}\theta_v\mathrm{d}\varphi_v\mathrm{d}\Phi_1\mathrm{d}\Phi_2 \tag{85}$$

$$1 \le s_i \le \infty, \quad -1 \le t_i \le 1, \quad 0 \le v \le \infty, \tag{86}$$

$$0 \le \theta_v \le \pi, \quad 0 \le \varphi_v \le 2\pi, \quad 0 \le \Phi_i \le 2\pi. \tag{87}$$

2) r_{ab} is Constant: In this case, the volume element is reduced to

$$\mathrm{d}\tau = \frac{v^6}{64}\left(s_1^2 - t_1^2\right)\left(s_2^2 - t_2^2\right)\mathrm{d}s_1\mathrm{d}s_2\mathrm{d}t_1\mathrm{d}t_2\mathrm{d}\Phi_1\mathrm{d}\Phi_2 \tag{88}$$

3.4. Trial Wavefunctions

The most suitable form of the trial wavefunctions for describing the four-body system is the one developed from Hilbert space components depending on Hylleraas' coordinates.

$$\left|\chi_j\right\rangle = s_1^{m_j} s_2^{n_j} \mathrm{e}^{-\alpha_j (s_1+s_2)} t_1^{k_j} t_2^{\ell_j} \cosh\left[\beta_j (t_1 - t_2)\right] u^{p_j} v^{q_j} \mathrm{e}^{-\gamma_j v}. \tag{89}$$

The total wavefunction of the system is then defined as the superposition of these components

$$\left|\Psi_k\right\rangle = \sum_{j=0}^{\infty} c_{kj} \left|\chi_j\right\rangle, \tag{90}$$

where k stands for the state of the system; $k=1$ identifies the ground-state, $k=2$ is the first excited state, etc. In practical calculations the number of superpositions is subjected to the convergence of the calculated energies and, therefore, limited to a certain value n.

Applying now the kinetic energy operators given at Equations (83) to the j-th component χ_j of the wavefunction, Equation (89), we obtain the following relations:

$$\begin{aligned}
T_1\chi_j = \frac{1}{v^2\left(s_1^2 - t_1^2\right)} \Bigg\{ & \Big[-4m_j\left(m_j-1\right) + 4k_j\left(k_j-1\right) - 4\left(p_j+2\right)\left(m_j-k_j\right) \\
& + 4\left(\alpha_j^2 - \beta_j^2\right)\Big] + \left[\frac{4m_j\left(m_j-1\right)}{s_1^2}\right] - \left[\frac{4k_j\left(k_j-1\right)}{t_1^2}\right] - \frac{8m_j\left(\alpha_j\right)}{s_1} \\
& - \frac{8k_j\left(\beta_j\right)}{t_1}\tanh\left[\beta_j\left(t_1-t_2\right)\right] + \left[4\alpha_j\left(2m_j+2+p_j\right)\right]s_1 \\
& + \left[4\beta_j\left(2k_j+2+p_j\right)\right]t_1\tanh\left[\beta_j\left(t_1-t_2\right)\right] - \left(4\alpha_j^2\right)s_1^2 \\
& + \left(4\beta_j^2\right)t_1^2 + \frac{\left(p_j\alpha_j\right)s_1^3}{u^2} + \frac{\left(p_j\beta_j\right)t_1^3}{u^2}\tanh\left[\beta_j\left(t_1-t_2\right)\right] \\
& - \left[\frac{p_j\left(m_j+p_j+k_j+1\right)s_1^2}{u^2}\right] + \left[\frac{p_j\left(m_j+p_j+k_j+1\right)t_1^2}{u^2}\right] \\
& - \frac{\left(p_j\alpha_j\right)s_1t_1^2}{u^2} - \frac{\left(p_j\beta_j\right)t_1s_1^2}{u^2}\tanh\left[\beta_j\left(t_1-t_2\right)\right] + \left[\frac{p_j\left(m_j-k_j\right)s_2^2}{u^2}\right] \\
& + \left[\frac{p_j\left(m_j-k_j\right)t_2^2}{u^2}\right] - \frac{\left(p_j\alpha_j\right)s_1s_2^2}{u^2} - \frac{\left(p_j\alpha_j\right)s_1t_2^2}{u^2} \\
& - \frac{\left(p_j\beta_j\right)t_1s_2^2}{u^2}\tanh\left[\beta_j\left(t_1-t_2\right)\right] - \frac{\left(p_j\beta_j\right)t_1t_2^2}{u^2}\tanh\left[\beta_j\left(t_1-t_2\right)\right] \\
& + \frac{\left(2p_j\beta_j\right)s_1s_2t_2}{u^2}\tanh\left[\beta_j\left(t_1-t_2\right)\right] + \frac{\left(2p_jk_j\right)s_1s_2t_2}{t_1u^2} \\
& + \frac{\left(2p_j\alpha_j\right)t_1s_2t_2}{u^2} - \frac{\left(2p_jm_j\right)t_1s_2t_2}{s_1u^2}\Bigg\}\chi_j,
\end{aligned} \tag{91a}$$

$$
\begin{aligned}
T_2\chi_j = \frac{1}{v^2\left(s_2^2 - t_2^2\right)}\Bigg\{ & \Big[-4n_j\left(n_j-1\right)+4l_j\left(l_j-1\right)-4\left(p_j+2\right)\left(n_j-l_j\right) \\
& +4\left(\alpha_j^2-\beta_j^2\right)\Big]+\left[\frac{4n_j\left(n_j-1\right)}{s_2{}^2}\right]-\left[\frac{4l_j\left(l_j-1\right)}{t_2{}^2}\right]-\frac{8n_j\left(\alpha_j\right)}{s_2} \\
& -\frac{8l_j\left(\beta_j\right)}{t_2}\tanh\left[\beta_j\left(t_1-t_2\right)\right]+\left[4\alpha_j\left(2n_j+2+p_j\right)\right]s_2 \\
& -\left[\frac{p_j\left(n_j+p_j+l_j+1\right)s_2^2}{u^2}\right]+\left[\frac{p_j\left(n_j+p_j+l_j+1\right)t_2^2}{u^2}\right] \\
& -\frac{\left(p_j\alpha_j\right)s_2t_2^2}{u^2}-\frac{\left(p_j\beta_j\right)t_2s_2^2}{u^2}\tanh\left[\beta_j\left(t_1-t_2\right)\right]+\left[\frac{p_j\left(n_j-l_j\right)s_1^2}{u^2}\right] \\
& +\left[\frac{p_j\left(n_j-l_j\right)t_1^2}{u^2}\right]-\frac{\left(p_j\alpha_j\right)s_2s_1^2}{u^2}-\frac{\left(p_j\alpha_j\right)s_2t_1^2}{u^2} \\
& +\frac{\left(p_j\beta_j\right)t_2s_1^2}{u^2}\tanh\left[\beta_j\left(t_1-t_2\right)\right]+\frac{\left(p_j\beta_j\right)t_2t_1^2}{u^2}\tanh\left[\beta_j\left(t_1-t_2\right)\right] \\
& -\frac{\left(2p_j\beta_j\right)s_1s_2t_1}{u^2}\tanh\left[\beta_j\left(t_1-t_2\right)\right]+\frac{\left(2p_jl_j\right)s_1s_2t_1}{t_2u^2} \\
& +\frac{\left(2p_j\alpha_j\right)t_1s_1t_2}{u^2}-\frac{\left(2p_jn_j\right)t_1s_1t_2}{s_2u^2}\Bigg\}\chi_j,
\end{aligned}
\tag{91b}
$$

Now, we deal with our system through the coordinates s_1, s_2, t_1, t_2, u, v rather than s_a, s_b, t_a, t_b, u, v. We notice from Equations (91) that T_a and T_b are obtained from T_1 and T_2, respectively, by replacing s_1, s_2, t_1, t_2, u, v by s_a, s_b, t_a, t_b, u, v, respectively. Thus, $T_a\chi_j$ and $T_b\chi_j$ can be derived via (91a) and (91b), respectively, using the same rearrangement.

Finally, from (84), applying the potential energy operator to the *j*-th component of the wavefunction, Equation (89), we find

$$
V_{\chi_j} = \frac{2}{v}\left[\left(\frac{1}{u}+1\right)-\frac{4s_1}{s_1{}^2-t_1{}^2}-\frac{4s_2}{s_2{}^2-t_2{}^2}\right]\chi_j \tag{91c}
$$

The forms of the matrix elements required for RRVM or VT are quite complicated and will not be presented here.

4. Results and Discussion

The computational part of the work has one main goal, namely, to test the possible existence and formation of four-body systems built up from electrons, positrons, protons, antiprotons muons antimuons, pions and antipions. Thus, we are seeking information about possible coexistences of matter and antimatter which would shed light on the relation between universe and antiuniverse.

The first step in the calculations is to optimize the parameters α, β, and γ involved in the wavefunction Equation (89) with respect to the energy. Many in-

vestigations have been carried out in this direction for each four-body system considered. The second step is to test the quality of the calculated binding energies when the number of superpositions (n) is increased. (The components of the wavefunction are obtained by selecting different values of the indices m_j, n_j, k_j, l_j, p_j and q_j and ignoring functions of the same symmetry). It has been shown that, monotonic convergence could be achieved with increasing n and $n = 25$ are adequate for obtaining excellent convergence.

4.1. Binding Energies of Heterohydrogen Molecules

In the present work a heteromolecule is defined as a molecule composed of an atom and its antiatom. Thus, heterohydrogen is the bound states of hydrogen and antihydrogen atoms ([49] [50]) which corresponds to case I defined at Equation (4), with $m_1 = m_a = m_e$ and $m_2 = m_b = M$ and m_e is the electronic mass, taken equals 1/2 in Hartree a.u. The reduced masses, Equation (3), reduced to $\mu_{12} = \mu_{ab} = m_e$ and M is set to be infinite. The threshold energy is now given by $E_{thr} = -1$ Hartree $= -27.2$ eV. Thus, Equation (8b) state that $\varepsilon(\sigma) = E(\sigma)$, and $\omega(\sigma) = W(\sigma)$. The optimization of the nonlinear parameters of the wavefunction provided us with $\alpha = 1.95$, $\beta = 0.87$ and $\gamma = 1.53$ when the first five components of the wavefunction (see Table 1) are considered.

Table 1. Components of the wavefunction defined at Equation (89).

j	m_j	n_j	k_j	ℓ_j	q_j	p_j
1	0	0	0	0	0	0
2	0	0	0	0	1	0
3	0	0	0	0	2	0
4	0	0	1	1	0	0
5	0	0	1	1	1	0
6	0	0	2	2	0	0
7	0	0	2	2	1	0
8	1	1	0	0	0	0
9	1	1	0	0	1	0
10	1	1	1	1	0	0
11	1	1	1	1	1	0
12	1	1	2	2	0	0
13	1	1	2	2	1	0
14	0	0	0	0	3	0
15	0	0	1	1	2	0
16	0	0	2	2	2	0
17	1	1	0	0	2	0
18	1	1	1	1	2	0
19	1	1	2	2	2	0
20	0	0	1	1	3	0
21	0	0	2	2	3	0
22	1	1	0	0	3	0
23	1	1	1	1	3	0
24	1	1	2	2	3	0
25	0	0	0	0	4	0

With these values, the convergence of the total and binding energies of the ground-state of the heterohydrogen was investigated. The binding energy obtained using 25 components of the wave function was found to be equal to −0.7476 eV. This result is in complete argument with the extension of the theorem of four-body systems. The stability of this molecule against dissociation to the lowest threshold state will be discussed in the next subsection.

The above investigations have been extended to other four-body systems for which case I, Equation (4), is valid and σ (=m/M) is changing between 0 and 1. In this case the stability of the systems is tested against dissociation into pairs of atoms and antiatoms possessing the same mass ratios (σ). The results of these investigations are displayed in Figure 4.

The Figure illustrates the monotonic behavior of the binding energy as a function of the mass ratio σ, which agrees completely with the prediction presented in Figure 2 and confirms the possible formation of the four-body systems.

4.2. Binding Energies of Positroniums with Protoniums, Muoniums and Pioniums

The results of the preceding section encourage the search for other four-body systems with internal clusters supported by case II, Equations (5), *i.e.* searching for exotic molecules stable against dissociation into light and heavy pairs. The most interesting systems [51] are those in which a positronium (Ps) is bound to a protonium (Pn), true muonium (Mu) or pionium ($A_{2\pi}$) exotic atoms. As a matter of fact, Pn, Mu and $A_{2\pi}$ have been synthesized very recently at CERN Laboratory (see [37] [38] [39], respectively). Thus, in addition to the positronium, the lastly mentioned works confirm the possible construction of other three

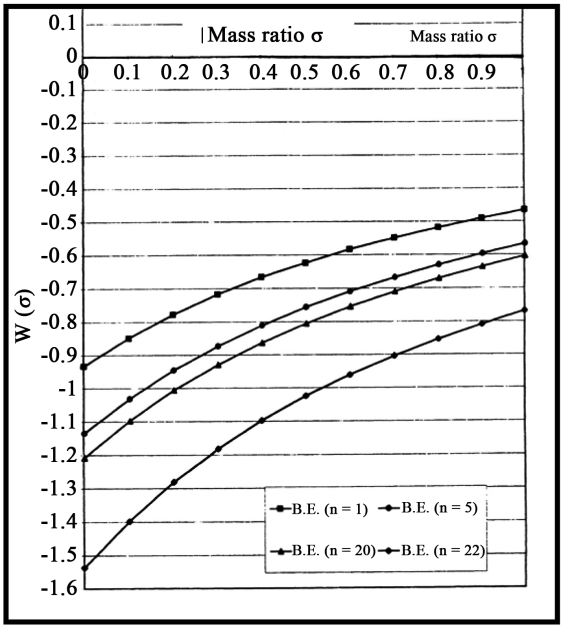

Figure 4. Convergence of the binding energies of four-body systems W(σ) with the increase of the number of superpositions (n) at different values of σ.

exotic atoms composed of particles and antiparticles. It has been shown that Pn is a neutral boson with zero baryon number, mean lifetime $\tau \sim 1.0 \times 10^{-6}$ s and ground state energy −12485.845 eV. On the other hand, the true muonium Mu is made up of two leptons, a muon, μ^-, and an antimuon μ^+. The binding energy of this exotic atom [38] is equal to −1407 eV (which is very close to the theoretical value −1406.024 eV). It is formed in triplet state (ortho-muonium) with lifetime 1.81×10^{-12} s and in singlet state (para-muonium) with lifetime 0.602×10^{-12} s eV. (True muonium should be distinguished from muonium atom which is a bound state composed of an electron and a positive muon). Nevertheless, it has been shown [39] that pionium, a bound state composed of two bosons; a pion, π^+, and an antipion π^-, possesses a binding energy equals −1860 eV (which is very close to the theoretical value −1898.56 eV), and a lifetime 2.89×10^{-15} s.

The first interesting system is the one composed of e^-, e^+, p^- and p^+. The lowest dissociation channel of this system is consisting of a positronium (Ps) and a protonium (Pn), with threshold energy E_{thr} = −12,492.28 eV. The rigorous mathematical proof of the existence of such system is given in Section 3.3 under the consideration of Equations (41a), (61) and (62). To show that the four particle system could form a bound state stable against dissociation to a pair of positronium and protonium exotic atoms, the Hamiltonian (1) and the wavefunction (89)-(90), are employed within the context of Rayleigh-Ritz' variational method discussed in Section 2.2. A set of 25 components have been employed for developing the trial wavefunction. Diagonalization of the Hamiltonian and optimization of the nonlinear parameters provided us with (see Equations (8a, b), $\omega(\sigma)$ = 0.000075 and total energy = −12,493.217 eV, *i.e.* the four body system has a binding energy $W(\sigma)$ = −0.9369 eV. This result indicates that the four body system e^-, e^+, p^- and p^+ is stable against dissociation to a positronium and a protonium. Thus, on considering the results obtained in the preceding section we remark that $\bar{H}H$ is stable against dissociation of any kind. Replacing the proton mass in the previous investigation with $2m_{p^+}$ and $3m_{p^+}$ allowed us to test whether $\bar{H}D$ and $\bar{H}T$, respectively, are stable against their dissociation to their lowest possible thresholds. The decisive answer to this question is demonstrated in **Table 2** (rows number 6 and 7, respectively). Thus, the present investigations confirm, for the first time, that all Hydrogen-Antihydrogen Molecules [41] [50] [51] [52] are stable against dissociation of any kind. A conclusion which should end contradicted arguments raised in the literature mainly by authors who prefer the treatment of four-body systems via Born-Oppenheimer approximations (see for example [53] [54] [55] [56]).

Our second goal in this section is focused on the characteristics of the variational energies calculated for other four body systems. Again, our main interest here is to test their stabilities against dissociation to the lowest possible channels, *i.e.* the positronium-true-muonium and positronium-pionium channels, respectively. Quite elaborate investigations using the same basis set employed in the preceding studies have shown that the total variational ground state energies of

Table 2. Total, Threshold and binding energies of various four-body systems.

System	Lowest Channel	α	β	γ	$\sigma = m/M$	E (eV)	$\omega(\sigma)$	$W(\sigma) = E_b$ (eV)	E_{thr} (eV)
$e^- e^+ e^+ e^-$	2Ps	1.95	0.87	1.53	1.0	−14.0352	0.0320	−0.4352	−13.6
$e^- e^+ \mu^- \mu^+$	Ps-Mu	3.02	0.03	1.08	0.005	−1415.6694	0.00197	−2.8451	−1412.8243
$e^- e^+ \pi^- \pi^+$	Ps-$A_{2\pi}$	3.18	0.03	2.03	0.004	−1907.225	0.000979	−1.8659	−1905.36
$e^- e^+ p^- p^+$	Ps-Pn	1.95	0.87	1.53	0.000545	−12493.217	0.000075	−0.9369	−12492.28
$e^- e^+ p^- d^+$	Ps-p^-d^+	1.95	0.87	1.53	0.000408	−16655.531	0.0000563	−0.94099	−16654.59
$e^- e^+ p^- t^+$	Ps-p^-t^+	1.95	0.87	1.53	0.000363	−18736.505	0.0000501	−0.93780	−18735.567
$\mu^- \mu^+ \pi^- \pi^+$	Mu-$A_{2\pi}$	1.40	0.05	1.82	0.757	−3407.003	0.0310	−102.419	−3304.584

the two systems are −1447.161 eV and −1907.225 eV, respectively. Knowing that E_{thr}(Ps Mu) = −1412.824 eV and E_{thr}(Ps $A_{2\pi}$) = −1905.36 eV, we realize (see rows 3 and 4, in Table 2), that the binding energies of both systems are W(Ps Mu) = −2.7852 eV and W(Ps $A_{2\pi}$) = −1.8276 eV, *i.e.* the systems are bound against dissociation to light (Ps) and heavy (Mu or $A_{2\pi}$) quasi atoms. Consequently, the four-body systems $e^- e^+ \mu^- \mu^+$ and $e^- e^+ \pi^- \pi^+$, are stable against dissociation of any kind.

Remember that $\omega(\sigma)$ is the shift below the threshold which is defined through the relation $E_g = (1+\omega(\sigma))E_{th}$, where E_{th} is the sum of the binding energies of the dissociated clusters 12 and ab and E_g stands for the total ground state energy of the corresponding four-body system. It is obvious that the inequality $\omega(\sigma) \leq \omega(1)$ is always fulfilled. Rows 6 and 7 contain information about the quasi molecules Ps-p^-d^+ and Ps-p^-t^+, respectively. The bottom raw in Table 2 contains the results of our investigations of the four-body system $\mu^- \mu^+ \pi^- \pi^+$. They show that the system is stable against dissociation into true muonium and pionium exotic atoms.

5. Implications of the Numerical Results

Since Hydrogen is the basic element of our universe (world) and the fusion of its atoms to Helium is the main process on Stars and Galaxies, the synthesizing of Antihydrogens and Antiheliums could be considered as strong supportive argument for the existence antiuniverse (Antiuniverse). The present section is devoted to the discussion of different ideas which could be considered as results of our numerical treatments of various four-body systems. Particularly, we are interested in their implementation in the universe-antiuniverse complex as suggested by the Big Bang theory (see Section 1), and in initiating fusion processes based on matter-antimatter annihilation.

5.1. Coexistence of Universe and Antiuniverse

One of the curious puzzles of Astrophysics is the observation of strong γ-radiations inform of ball lightning at distance considered as the edges of our universe (Ashby and Whitehead [53], see also [54] [55] [56] [57]), and the appearance of

isotopic cosmic background spectrum of Gamma-rays above 1 MeV (David and Huges [58], see also [59]). The formation of exotic atoms at CERN composted of particles and antiparticles as well as the possible formation of different four-body systems (Section 4) support the possible coexistence of matter and antimatter. Thus, suggesting the possible existence of an overlap area between the universe and antiuniverse. With regarding to the origin of our universe, it seems that matter and antimatter were attracted immediately after the big bang to different centers of gravity, a process which led to relatively rapid cooling and construction of not completely separated universe and antiuniverse. This argument could also explain a recent discovery that cosmic rays are mainly composed of particles and antiparticles [60] [61] [62] [63].

5.2. Cold Fusion

The possible formation of Hydrogen-Antihydrogen Molecules allows us to propose the following scenario for implementation in cold fusion which is alternative to a suggestion made by Fleischmann and Pons [64] [65]. In our case (see also [66] [67]), we argue that if a thermalized beam of antihydrogens passes through a palladium sheet in which hydrogen (deuterium or tritium), atoms are localized, a bound-state (or quazimolecular structure) could be formed. Additionally, if the antihydrogen enters the Coulomb barrier of the localized atom, the system could collapse in two different channels, namely the annihilation and fusion channels yielding to huge amount of energy which could be considered as promising alternatives to nuclear energy sources based on nuclear fission and fusion processes.

6. Conclusions

The main goal of the present paper was to provide the mathematical proof of the possible formation in nature of quasi molecular structures composed of matter and antimatter. In order to confirm computationally the result of the theory, a computer code was established based on Ritz' variational method. Quite elaborate calculations were performed using Hylleraas type wavefunctions.

The most interesting conclusions of the present work can be summarized in the following points:

1) The resultant calculations confirm for the first time the stability of heterohydrogens against dissociation to positronium and protonium (deuterium or tritium) atoms. Also, the possible formation in nature of positronium-muonium and positronium-pionium compounds was established for the first time.

2) The possible coexistence of matter and antimatter is a reliable reasoning for possible existence of an overlap area between universe and antiuniverse, a matter which could act against the assumption about existing asymmetry immediately after the occurrence of the Big Bang.

3) Coexistence of matter-antimatter systems suggests the possible existence of fusion channels applied to produce huge amount of energy.

4) Formation of matter-antimatter molecular compounds should open the

gate in front of a new field of Chemistry to be referred to as "Antimatter Chemistry". This may lead to new ideas about the nature of global chemical bonds.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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