

Investigation of the Stability of Some Exotic Four Particle Systems

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Abstract. Possible existence of exotic molecules consisting of $N=4$ unit charge particles is investigated using the Rayleigh-Ritz variational method. Several exotic molecules of the form $A^-B^+B^-A^+$ ($e^-\mu^+\mu^-e^+$, $e^-\pi^+\pi^-e^+$, and $\mu^-\pi^+\pi^-\mu^+$) are found to exist as bound states.

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1 Introduction

The question about the existence of exotic molecules has become very important. Several systems of unit charge particles have been recently studied. The simplest of these systems are the positronium ion ($e^+e^-e^-$) predicted by Wheeler [1] and experimentally observed by Mills [2], the Ps_2 molecule ($e^-e^+e^-e^+$) and the PsH system predicted by Hylleraas and Ore [3]. These systems have been extensively studied recently by various theoretical methods [4].

The problem of stability of hydrogen-antihydrogen molecule is of particular interest, since this is the simplest matter-antimatter molecular structure, and may be considered fundamental in a theoretical investigation of the stability of many exotic systems. This problem was treated many years ago by many authors [5–7]. Recently, Richard [8, 9] showed that the stability domain of the systems made up of four particles, two having the same positive charge and two having the opposite negative charge, interacting only through coulombic forces, could be represented in terms of points in the interior, or on the surface, of a regular tetrahedron. Following this idea, Armour et. al. [10] showed that $H\bar{H}$ lies deeply inside the domain of instability. Gridnev and Greiner [11] have explained the instability of $H\bar{H}$ through the screening effect of the heavy p (\bar{p}), so that the bieletrons see the tightly bound pair ($p\bar{p}$) as neutral and the system falls apart.

On the other hand, Abdel-Raouf and Ladik [12] have proved that the binding energy W which binds the atom and antiatom together in the four particle-antiparticle system ($m_1^-, m_2^+, m_1^+, m_2^-$) is a monotonic function of the mass

ratio σ characterizing the (m_1, m_2) atomic system within the σ interval $[0,1]$, and satisfying the relation

$$W(0) \leq W(\sigma) \leq W(1) \quad \forall \sigma \in [0, 1]$$

which implies the negativity of $W(\sigma)$ for all $\sigma \in [0, 1)$ if $W(1)$ is negative. This in consequence means that the existence of positronium molecule, $\sigma = 1$, is sufficient to predict the existence of $H\bar{H}$ molecule, $\sigma = 0$, and also all similar exotic molecules with $\sigma \in (0, 1)$. Accordingly, systems like $e^-\mu^+\mu^-e^+$, $e^-\pi^+\pi^-e^+$,..... could also exist.

In this work the systems $e^-\mu^+\mu^-e^+$, $e^-\pi^+\pi^-e^+$ and $\mu^-\pi^+\pi^-\mu^+$ will be tested. Rayleigh-Ritz variational technique is used to predict upper bounds for the energies of the systems. In Section 2, the theoretical treatment of the four particle systems is discussed and the Rayleigh-Ritz variational method is reviewed. In Section 3, the Hylleraas coordinates for the systems are defined, the wave function is introduced and the the integrals of the matrix components are treated. Results are listed in Section 4, and conclusions drawn are summarized in Section 5.

2 Treatment of the Four Particle Systems

A quasimolecular structure consisting of two particles and two antiparticles is governed by the Hamiltonian

$$H = \sum_{i=1}^4 \frac{-\hbar^2}{2m_i} \nabla_i^2 + \sum_{i < j}^4 \frac{q_i q_j}{|\vec{r}_i - \vec{r}_j|}. \quad (1)$$

The particles are considered to have unit charge, that is $|q_i| = 1$. Using

$$\nabla_i^2 = \sum_{j \neq i} \left(\nabla_i \frac{\partial}{\partial r_{ij}} \right) \cdot \hat{r}_{ij} + (\nabla_i \cdot \hat{r}_{ij}) \frac{\partial}{\partial r_{ij}}, \quad (2)$$

where the first of these terms is given by

$$\sum_{j \neq i} \left(\nabla_i \frac{\partial}{\partial r_{ij}} \right) \cdot \hat{r}_{ij} = \sum_{j \neq i} \frac{\partial^2}{\partial r_{ij}^2} + 2 \sum_{\substack{j,k \neq i \\ j < k}} \cos \theta_{ij,ik} \frac{\partial^2}{\partial r_{ij} \partial r_{ik}} \quad (3)$$

with

$$\cos \theta_{ij,ik} = \frac{r_{ij}^2 + r_{ik}^2 - r_{jk}^2}{2r_{ij}r_{ik}} \quad (4)$$

the Hamiltonian (1) can be written as

$$H = \sum_{i=1}^4 \frac{-\hbar^2}{2m_i} \sum_{j \neq i} \left(\frac{\partial^2}{\partial r_{ij}^2} + \frac{2}{r_{ij}} \frac{\partial}{\partial r_{ij}} + 2 \sum_{k>j} \cos \theta_{ij,ik} \frac{\partial^2}{\partial r_{ij} \partial r_{ik}} \right) + \sum_{i<j}^4 \frac{q_i q_j}{r_{ij}} \quad (5)$$

It is well known that there is no closed-form analytical solution to the four-particle eigenvalue problem. Hence, the energy is most accurately obtained by variational minimization of the energy functional $E[\Psi]$ defined as

$$E[\Psi] = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \quad (6)$$

with respect to the parameters in the wave function. The Rayleigh-Ritz variational method proved to be suitable in performing these calculations [13]. According to this technique, a trial wave function $|\psi_t^n\rangle$ is expanded in Hilbert space of dimension n in the form

$$|\psi_t^n\rangle = \sum_k^n a_k |\psi_{tk}\rangle, \quad (7)$$

so that

$$\langle \psi_{tk}^n | \psi_{tk'}^n \rangle = \delta_{kk'}; \quad k \& k' = 1, 2, \dots, n. \quad (8)$$

On the other hand, all trial functions $|\psi_{tk}^n\rangle$ must be generated from a complete set of basis functions $|\chi_i\rangle$ which expanding the H-domain of the molecule considered

$$|\psi_{tk}^n\rangle = \sum_{i=1}^n c_{ki} |\chi_i\rangle. \quad (9)$$

Normally, the application of the variational principle will result in a set of secular equations for each state, k , of the system

$$\sum_{j=1}^n c_{kj} [\langle \chi_i | H | \chi_j \rangle - E_{nk} \langle \chi_i | \chi_j \rangle] = 0; \quad i = 1, 2, \dots, n, \quad (10)$$

and the eigenenergies are obtained from

$$\det (H_{ij} - E_{nk} S_{ij}) = 0, \quad (11)$$

where

$$H_{ij} = \langle \chi_i | H | \chi_j \rangle, \quad (12)$$

and

$$S_{ij} = \langle \chi_i | \chi_j \rangle. \quad (13)$$

Rayleigh [14] and Ritz [15] proved the relation

$$E_1 \leq E_1^n; \quad n \succ 0, \quad (14)$$

which asserts that the variational ground state energy is an upper bound to the exact one. Moreover, Hylleraas and Undheim [16], proved that the relation

$$E_k \leq E_k^n; \quad k = 1, 2, \dots, n \quad (15)$$

is satisfied provided that Eq. (7) is fulfilled. Relations (14) and (15) in turn state that all variational E_k^n are upper bounds to the exact $|E_k\rangle$'s.

3 Description of the Method

3.1 The Hylleraas coordinates

The Hylleraas coordinates are natural coordinates for treating the four body systems [17–19]. These coordinates are defined as the following:

$$s_i = \frac{(r_{ia} + r_{ib})}{r_{ab}}; \quad i = 1, 2 \quad (16)$$

$$t_i = \frac{(r_{ia} - r_{ib})}{r_{ab}}; \quad i = 1, 2 \quad (17)$$

$$s_a = \frac{(r_{1a} + r_{2a})}{r_{12}}, \quad s_b = \frac{(r_{1b} + r_{2b})}{r_{12}} \quad (18)$$

$$t_a = \frac{(r_{1a} - r_{2a})}{r_{12}}, \quad t_b = \frac{(r_{1b} - r_{2b})}{r_{12}} \quad (19)$$

$$u = \frac{r_{12}}{r_{ab}}, \quad v = r_{ab} \quad (20)$$

$$\cos \theta_{ia,ib} = \frac{s_i^2 + t_i^2 - 2}{s_i^2 - t_i^2}, \quad (21)$$

where 1 and 2 are the two negatively charged particles, while a and b are the two positively charged particles. The Hamiltonian terms of Eq. (5) are given in these coordinates by the following expressions:

$$\begin{aligned} \nabla_1^2 = & \frac{4}{v^2} \frac{1}{s_1^2 - t_1^2} \left[(s_1^2 - 1) \frac{\partial^2}{\partial s_1^2} + (1 - t_1^2) \frac{\partial^2}{\partial t_1^2} + 2s_1 \frac{\partial}{\partial s_1} - 2t_1 \frac{\partial}{\partial t_1} \right] \\ & - \frac{1}{v^2} \left[\frac{\partial}{\partial u} + \frac{2}{u} + 2(\cos \theta_{12,1a} + \cos \theta_{12,1b}) \frac{\partial}{\partial s_1} \right. \\ & \left. + 2(\cos \theta_{12,1a} - \cos \theta_{12,1b}) \frac{\partial}{\partial t_1} \right] \frac{\partial}{\partial u} \quad (22) \end{aligned}$$

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$$\begin{aligned} \nabla_2^2 = & \frac{4}{v^2} \frac{1}{s_2^2 - t_2^2} \left[(s_2^2 - 1) \frac{\partial^2}{\partial s_2^2} + (1 - t_2^2) \frac{\partial^2}{\partial t_2^2} + 2s_2 \frac{\partial}{\partial s_2} - 2t_2 \frac{\partial}{\partial t_2} \right] \\ & - \frac{1}{v^2} \left[\frac{\partial}{\partial u} + \frac{2}{u} + 2(\cos \theta_{12,2a} + \cos \theta_{12,2b}) \frac{\partial}{\partial s_2} \right. \\ & \left. + 2(\cos \theta_{12,2a} - \cos \theta_{12,2b}) \frac{\partial}{\partial t_2} \right] \frac{\partial}{\partial u} \quad (23) \end{aligned}$$

$$\begin{aligned} \nabla_a^2 = & \frac{4}{u^2 v^2} \frac{1}{s_a^2 - t_a^2} \left[(s_a^2 - 1) \frac{\partial^2}{\partial s_a^2} + (1 - t_a^2) \frac{\partial^2}{\partial t_a^2} + 2s_a \frac{\partial}{\partial s_a} - 2t_a \frac{\partial}{\partial t_a} \right] \\ & - \left[\frac{\partial}{\partial v} + \frac{2}{v} + \frac{2}{uv} (\cos \theta_{1a,ab} + \cos \theta_{2a,ab}) \frac{\partial}{\partial s_a} \right. \\ & \left. + \frac{2}{uv} (\cos \theta_{1a,ab} - \cos \theta_{2a,ab}) \frac{\partial}{\partial t_a} \right] \frac{\partial}{\partial v} \quad (24) \end{aligned}$$

$$\begin{aligned} \nabla_b^2 = & \frac{4}{u^2 v^2} \frac{1}{s_b^2 - t_b^2} \left[(s_b^2 - 1) \frac{\partial^2}{\partial s_b^2} + (1 - t_b^2) \frac{\partial^2}{\partial t_b^2} + 2s_b \frac{\partial}{\partial s_b} - 2t_b \frac{\partial}{\partial t_b} \right] \\ & - \left[\frac{\partial}{\partial v} + \frac{2}{v} + \frac{2}{uv} (\cos \theta_{1b,ab} + \cos \theta_{2b,ab}) \frac{\partial}{\partial s_b} \right. \\ & \left. + \frac{2}{uv} (\cos \theta_{1b,ab} - \cos \theta_{2b,ab}) \frac{\partial}{\partial t_b} \right] \frac{\partial}{\partial v} \quad (25) \end{aligned}$$

$$V = \frac{2}{v} \left[\left(\frac{1}{u} + 1 \right) - \frac{4s_1}{s_1^2 - t_1^2} - \frac{4s_2}{s_2^2 - t_2^2} \right] \quad (26)$$

3.2 Construction of the trial wave function

Since the only practical way to calculate the energy and properties of the four-particle systems is to use variational approach, one needs a (good) wave function which to be able to give accurate results. A suitable correlated wave function is that used by James and Coolidge for H_2 molecule [19]

$$|\chi_j\rangle = \left(s_1^{m_j} s_2^{n_j} t_1^{k_j} t_2^{l_j} + s_1^{n_j} s_2^{m_j} t_1^{l_j} t_2^{k_j} \right) e^{-\alpha(s_1+s_2)u^{p_j}}. \quad (27)$$

This function has the advantage of satisfying the symmetric property of the molecule under the exchange of particles and antiparticles. Besides, it has its power in the many variational coefficients which can be adjusted to yield accurate results for diatomic molecules. However, unlike real wave functions, James and Coolidge wave function does not satisfy the correlation cusp condition, while the physical insight about molecular bonding seems to be lost. In addition, for large s_1 and s_2 , the asymptotic conditions are violated [20]. A

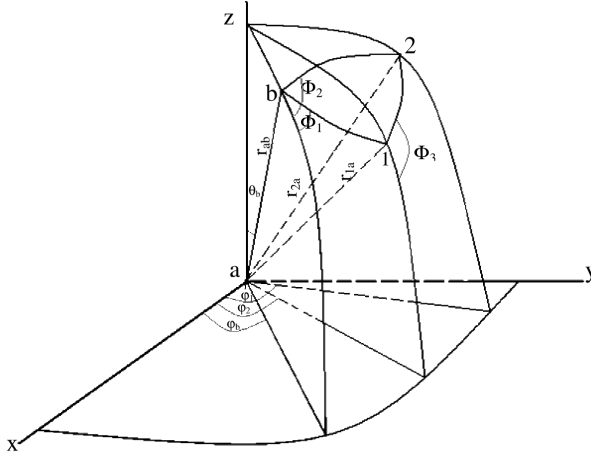


Figure 1. Geometrical Representation of the Four-Particle System.

better approach is obtained if the wave function describes all possible ionic behavior besides the covalent characteristics of the molecule [3], while explicitly including a correlation function $f(r_{ab})$ to avoid Born-Oppenheimer approximation for the atom-antiatom systems under consideration. A wave function which can meet these conditions besides satisfying both limits adequately is the following:

$$|\chi_j\rangle = s_1^{m_j} s_2^{n_j} t_1^{k_j} t_2^{l_j} e^{-\alpha(s_1+s_2)} \cosh[\beta(t_1 - t_2)] u^{p_j} v^{q_j} e^{-\gamma v}. \quad (28)$$

3.3 Integrals in s, t, u and v

The volume element of the system is obtained in terms of its relative coordinates, Figure 1, as [21,22]

$$\begin{aligned} d\tau &= r_{ab}^2 r_{1a}^2 r_{2a}^2 \sin \theta_b \sin \theta_1 \sin \theta_2 dr_{ab} dr_{1a} dr_{2a} d\theta_b d\theta_1 d\theta_2 d\varphi_b d\varphi_1 d\varphi_2 \\ &= r_{1a}^2 r_{2a}^2 r_{ab}^2 dr_{1a} dr_{2a} dr_{ab} J(\theta_{1b}, \theta_{2b}, \theta_b, \Phi_1, \Phi_2, \varphi_b) \\ &\quad \times \sin \theta_1 \sin \theta_2 \sin \theta_b d\theta_{1b} d\theta_{2b} d\theta_b d\Phi_1 d\Phi_2 d\varphi_b \quad (29) \end{aligned}$$

Considering r_{ab} to be the axis of rotation of the molecule, the volume element can then be written as

$$\begin{aligned} d\tau &= r_{1a} r_{2a} r_{1b} r_{2b} dr_{1a} dr_{2a} dr_{1b} dr_{2b} dr_{ab} \sin \theta_b d\theta_b d\varphi_b d\Phi_1 d\Phi_2 \\ &= J(s_1, s_2, t_1, t_2) (s_1^2 - t_1^2) (s_2^2 - t_2^2) \frac{v^4}{16} ds_1 ds_2 dt_1 dt_2 dv \sin \theta_v d\theta_v d\varphi_v d\Phi_1 d\Phi_2 \\ &= \frac{1}{64} (s_1^2 - t_1^2) (s_2^2 - t_2^2) v^8 ds_1 ds_2 dt_1 dt_2 dv \sin \theta_v d\theta_v d\varphi_v d\Phi_1 d\Phi_2 \quad (30) \end{aligned}$$

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Accordingly the integration of any integrand f , which is a function of (s, t, u, v) will be given by

$$\int f d\tau = \frac{1}{64} \int (s_1^2 - t_1^2) (s_2^2 - t_2^2) ds_1 ds_2 dt_1 dt_2 d\Phi_1 d\Phi_2 \times \int f(s, t, u, v) v^8 dv \sin \theta_v d\theta_v d\varphi_v, \quad (31)$$

where

$$\begin{aligned} 1 \leq s_i \leq \infty, & \quad -1 \leq t_i \leq 1, & \quad 0 \leq v \leq \infty \\ 0 \leq \theta_v \leq \pi, & \quad 0 \leq \varphi_v \leq 2\pi, & \quad 0 \leq \Phi_i \leq 2\pi \end{aligned}$$

The function $f(s, t, u, v)$ could be $\psi H \psi$ or ψ^2 , so that the integration of Eq. (31) will have the general form

$$\begin{aligned} & \frac{1}{64} \int (s_1^2 - t_1^2) (s_2^2 - t_2^2) g(s, t) s_1^m s_2^n t_1^k t_2^l u^p e^{-\delta(s_1+s_2)} \\ & \times \begin{cases} \cosh^2[\beta(t_1 - t_2)] \\ \cosh[\beta(t_1 - t_2)] \sinh[\beta(t_1 - t_2)] \end{cases} ds_1 ds_2 dt_1 dt_2 d\Phi_1 d\Phi_2 \\ & \times \int v^q dv \sin \theta_v d\theta_v d\varphi_v, \quad (32) \end{aligned}$$

where

$$g(s, t) = \begin{cases} \frac{1}{s_i^2 - t_i^2} & \text{as in } \nabla_i^2 \chi_j \\ 1 & \text{as in the matrix components of unity} \end{cases}. \quad (33)$$

On using

$$\begin{aligned} \cosh x &= \frac{1}{2} (e^x + e^{-x}) \\ \sinh x &= \frac{1}{2} (e^x - e^{-x}), \end{aligned} \quad (34)$$

and performing integration over v, θ_v and φ_v , the integral (32) gives

$$\begin{aligned} & \frac{\pi}{64} \frac{q!}{\gamma^{q+1}} [I_g(m, n, k, l, p, \delta, 2\beta) \pm I_g(m, n, k, l, p, \delta, -2\beta) \\ & \pm I_g(m, n, k, l, p, \delta, 0) + I_g(m, n, k, l, p, \delta, 0)], \quad (35) \end{aligned}$$

where the \pm stands for \cosh^2 and $\cosh \sinh$, respectively, while the integral I_g is given by

$$\begin{aligned} I_g(m, n, k, l, p, \delta, \eta) &= \int (s_1^2 - t_1^2) (s_2^2 - t_2^2) g(s, t) s_1^m s_2^n t_1^k t_2^l u^p e^{-\delta(s_1+s_2)} \\ & \times e^{\eta(t_1-t_2)} ds_1 ds_2 dt_1 dt_2 d\Phi_1 d\Phi_2, \quad (36) \end{aligned}$$

where η may be positive, negative or zero. Substituting with the form of $g(s, t)$ from Eq. (33) implies the following general integral form

$$I_p(m, n, k, l, \delta, \eta) = \int s_1^m s_2^n t_1^k t_2^l u^p e^{-\delta(s_1+s_2)} e^{\eta(t_1-t_2)} ds_1 ds_2 dt_1 dt_2 d\Phi_1 d\Phi_2 \quad (37)$$

In performing this integration, it is necessary to expand the powers of u in terms of other variables since u is not used directly as one of the variables of integration. This is achieved using the notation of James and Coolidge for u^2 [19], i.e.

$$u^2 = \frac{1}{4} \{ s_1^2 + s_2^2 + t_1^2 + t_2^2 - 2 - 2s_1s_2t_1t_2 - 2[(s_1^2 - 1)(s_2^2 - 1)(1 - t_1^2)(1 - t_2^2)]^{1/2} \cos(\Phi_1 - \Phi_2) \} \quad (38)$$

Besides the Neumann's expansion for u^{-1} [23,24], i.e.

$$\frac{1}{u} = 2 \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} F_{ij} P_i^j(s) Q_i^j(s) P_i^j(t_1) P_i^j(t_2) \cos[j(\Phi_1 - \Phi_2)] \quad (39)$$

with

$$F_{ij} = (-1)^j \times 2(2i+1) \left[\frac{(i+j)!}{(i-j)!} \right]^2; \quad j \succ 0 \quad (40)$$

$$F_{i0} = 2i + 1$$

where P_i^j and Q_i^j are the associated Legendre functions of the first and second kinds, respectively.

The solution of the integral I_p clearly depends on the value of the index p . The details of calculations of I_p at different values of p are given in the Appendix.

4 Calculations and Results

The solution of the integral I_p contains functions which are very sensitive to the computer accumulation error, like the functions Z_τ^μ and G_τ^μ appearing in equation (A.19). To overcome this problem extended precision is used and the calculations are made to a large number of significant figures. Besides, the exponential function e^x is evaluated through its Maclaurin expansion with an absolute error

$$\text{error} \Big|_{i=j} = \frac{x^j/j!}{\sum_{i=0}^{j-1} x^i/i!} \quad (41)$$

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set to 10^{-30} . On the other hand, the logarithmic function is evaluated from the Maclaurin expansion of

$$(1+x)^{15} \ln(1+x), \quad (42)$$

which gives

$$\ln(1+x) = (1+x)^{-15} \left\{ \sum_{i=0}^{15} a_i \frac{x^i}{i!} + \sum_{i=16}^{\infty} \frac{1}{i!} (-1)^i a_{16} (i-16)! \right\}; \quad (43)$$

$$0 < x < 1,$$

and

$$\ln(y) = k \ln(2) + \ln(z); \quad y > 2 \quad (44)$$

where

$$y = 2^k \times z. \quad (45)$$

The coefficients of expansion, a_i , are given in Table 1. They are exact and hand made calculated to avoid any approximation.

Table 1. Coefficients of Maclaurin expansion of Eq. (42)

i	a_i	i	a_i	i	a_i	i	a_i
1	1	5	140274	9	157689×10^4	13	11888257248×10^2
2	29	6	17631×10^2	10	112775544×10^2	14	30314886336×10^2
3	587	7	194715×10^2	11	672850584×10^2	15	43391630016×10^2
4	9774	8	1882044×10^2	12	3236266656×10^2	16	1307674368×10^3

The nonlinear parameters of the wave function, α , β and γ , are optimized to improve the correlation between particles in each molecule. Only one parameter is changed in a time to avoid local minima traps. The process is repeated for another parameter keeping those tested to be fixed at their optimum values, until finally all parameters are optimized so that the lowest energy is obtained.

A trial wave function composed of 5, 9, 15...21 terms is used. The ground state energies E_g corresponding to these terms are shown in Table 2 for the systems $e^- \mu^+ \mu^- e^+$, $e^- \pi^+ \pi^- e^+$, and $\mu^- \pi^+ \pi^- \mu^+$. The Table also shows calculations for the Ps_2 molecule which are made to test method and program. It can be seen that the result obtained for this molecule is compatible with that of other workers [25, 26].

It is apparent from the Table that E_g converges as the number of the wave function terms increases. The 21st-term considered is a term concerning the correlation between the two positive particles of the system, i.e., $p_j \neq 0$, which seems to adjust the ground state energy of the system.

In Table (3) the resulted ground state energies for each system are listed together with the fraction x of binding below threshold which is defined through the

Table 2. Ground state energies at different wave function terms.

[$m_j n_j k_j \ell_j q_j p_j$]	E_g a.u.			
	$e^- e^+ e^- e^+$	$e^- \mu^+ \mu^- e^+$	$e^- \pi^+ \pi^- e^+$	$\mu^- \pi^+ \pi^- \mu^+$
[000000]	-0.373			
[110000]				
[000010]				
[110010]				
[000020]	-0.4915	-2.6294	-2.728	-15.3973
[110020]				
[000030]				
[110030]				
[001100]	-0.5052			
[111100]		-4.6233	-4.6892	-119.9125
[001110]	-0.50805			
[111110]				
[002200]	-0.50975			
[112200]				
[002210]	-0.511727	-46.33517	-62.8936	-120.5357
[112210]		-52.7831	-69.4591	-120.5934
[001120]	-0.511728	-52.8569	-69.6196	-122.6603
[111120]		-53.0377	-69.7908	-122.705
[001130]		-53.2435	-70.3159	-123.0955
[111130]		-53.337	-70.491	-123.124
[000001]	-0.5160	-53.2045	-70.1186	-126.415

Table 3. The fraction x of binding below threshold for the systems.

System	α	β	γ	σ	E_g a.u.	x
$e^- e^+ e^- e^+$	1.950	0.87	1.53	1	-0.5160	0.0320
$e^- \mu^+ \mu^- e^+$	3.0180	0.03	1.08	0.00473	-53.20445	0.00197
$e^- \pi^+ \pi^- e^+$	3.181	0.03	2.025	0.003582	-70.1186	0.000979
$\mu^- \pi^+ \pi^- \mu^+$	1.4	0.05	1.82	0.75716	-126.4151	0.0307

relation

$$E_g = (1 + x) E_{th}. \quad (46)$$

The optimum values of the nonlinear parameters together with the mass ratio σ are also given for each system. The Table shows that the fraction x of binding below threshold is an increasing function of σ

$$x(\sigma) \leq x(1) \quad \text{for } \sigma \leq 1 \quad (47)$$

5 Conclusions

The most important conclusion of this work is the confirmation of the existence of systems under study. This supports the theory of Abdel-Raouf [27] for the existence of exotic molecules. Results show that the fraction x of binding below threshold is an increasing function of σ .

6 Appendix

The solution of the integral (37) is given below at different powers, p , of u .

6.1 $p = 0$

Upon integration over the azimuthal angles, the integral (37) for $p = 0$ will be given by

$$\begin{aligned} I_0(m, n, k, l, \delta, \eta) &= 4\pi^2 \int_1^\infty s_1^m e^{-\delta s_1} ds_1 \int_1^\infty s_2^n e^{-\delta s_2} ds_2 \int_{-1}^1 t_1^k e^{\eta t_1} dt_1 \int_{-1}^1 t_2^l e^{-\eta t_2} dt_2 \\ &= 4\pi^2 A_m(1, \delta) A_n(1, \delta) B_k(\eta) B_l(-\eta) \end{aligned} \quad (\text{A.1})$$

where the integrations A and B are defined as

$$A_l(a, b, \alpha) = \int_a^b \lambda^l e^{-\alpha \lambda} d\lambda \quad (\text{A.2})$$

and

$$B_\kappa(\pm\eta) = \int_{-1}^1 \lambda^\kappa e^{\pm\eta \lambda} d\lambda. \quad (\text{A.3})$$

The integral A is solved through integration by parts to yield the relation

$$A_l(a, b, \alpha) = \sum_{\mu=0}^l \frac{l!}{(l-\mu)!} \frac{1}{\alpha^{\mu+1}} [-\lambda^{\mu} e^{-\alpha \lambda}]_a^b. \quad (\text{A.4})$$

For $b = \infty$ we then have

$$A_l(a, \alpha) = \frac{e^{-a\alpha}}{\alpha} \sum_{\mu=0}^l \frac{l!}{(l-\mu)!} \frac{a^{\mu}}{\alpha^{\mu}}. \quad (\text{A.5})$$

The integral B , on the other hand, is solved using series expansion for the exponential function to give

$$B_{\kappa}(\pm\eta) = \begin{cases} \frac{2}{\kappa+1} + \sum_{\nu=1}^{\infty} \frac{2\eta^{2\nu}}{(2\nu)!(\kappa+2\nu+1)} & \text{for even } \kappa \\ \pm \sum_{\nu=0}^{\infty} \frac{2\eta^{2\nu+1}}{(2\nu+1)!(\kappa+2\nu+2)} & \text{for odd } \kappa \end{cases}. \quad (\text{A.6})$$

6.2 p is even

In this case, the expansion of u^p is obtained from the relation

$$u^p = (u^2)^{\nu}; \quad \nu = \frac{p}{2}, \quad (\text{A.7})$$

where u^2 is given by the relation (38). Using

$$\cos^r \theta = \left(\frac{1}{2}\right)^r \sum_{\kappa=0}^r \frac{r!}{\kappa!(r-\kappa)!} \cos(r-2\kappa)\theta. \quad (\text{A.8})$$

Upon integration over the azimuthal angles, all terms containing the cosine function will vanish except those for which $r = 2k$. Accordingly

$$\begin{aligned} & I_p(m, n, k, \ell, \delta, \eta) \\ &= 4\pi^2 \left(\frac{1}{4}\right)^{\nu} \sum_{\rho=0}^{\lambda} \frac{\nu!}{\left(\frac{\nu-\mu}{2}\right)!^2} \sum_{\kappa_1=0}^{\mu} \sum_{\kappa_2=0}^{\kappa_1} \sum_{\kappa_3=0}^{\kappa_2} \sum_{\kappa_4=0}^{\kappa_3} \sum_{\kappa_5=0}^{\kappa_4} \frac{(-2)^{\kappa_4}}{(\mu-\kappa_1)! \kappa_5!} \\ & \times \left(\prod_{i=1}^4 \frac{1}{(\kappa_i - \kappa_{i+1})!} \right) \sum_{\xi_1, \xi_2, \xi_3, \xi_4=0}^{(\nu-\mu)/2} \left[\prod_{j=1}^4 \frac{[(\nu-\mu)/2]!}{\xi_j! \left(\frac{\nu-\mu}{2} - \xi_j\right)!} \right] (-1)^{\nu-\mu-\xi_1-\xi_2+\xi_3+\xi_4} \\ & \times I_0(m+2\nu-2\kappa_1+2\xi_1+\kappa_5, n+2\kappa_1-2\kappa_2+2\xi_2+\kappa_5, k+2\kappa_2-2\kappa_3+2\xi_3+\kappa_5, \\ & \quad \ell+2\kappa_3-2\kappa_4+2\xi_4+\kappa_5, \delta, \eta) \quad (\text{A.9}) \end{aligned}$$

where λ is defined by

$$\lambda = \begin{cases} \nu/2 & \text{for even } \nu \\ (\nu-1)/2 & \text{for odd } \nu \end{cases}, \quad (\text{A.10})$$

while ν is defined by

$$\mu = \begin{cases} 2\rho & \text{for even } \nu \\ 2\rho+1 & \text{for odd } \nu \end{cases}, \quad (\text{A.11})$$

and I_0 is given by relation (A.1).

6.3 p is odd

The expansion of u^p is obtained from the relation

$$u^p = (u^2)^\nu u^{-1}; \quad \nu = \frac{p+1}{2}, \quad (\text{A.12})$$

where u^2 and u^{-1} are given by the relations (38) and (39), respectively. Using the relation

$$\begin{aligned} & \cos^\mu \theta \cos j\theta \\ &= \left(\frac{1}{2}\right)^{\mu+1} \sum_{\kappa=0}^{\mu} \frac{\mu!}{\kappa!(\mu-\kappa)!} [\cos(j-\mu+2\kappa)\theta + \cos(j+\mu-2\kappa)\theta] \end{aligned} \quad (\text{A.13})$$

and recall that upon integration over Φ_1 and Φ_2 all terms containing the cosine function will vanish except those for which the cosine argument is zero, relation (A.12) is written as

$$\begin{aligned} u^p &= \left(\frac{1}{2}\right)^{2\nu-1} \left[(s_1^2 + s_2^2 + t_1^2 + t_2^2 - 2 - 2s_1s_2t_1t_2)^\nu \right. \\ & \quad \times \sum_{i=0}^{\infty} F_{i0} P_i(s \prec) Q_i(s \succ) P_i(t_1) P_i(t_2) \left. \right] \\ & \quad + \left(\frac{1}{2}\right)^{2\nu-1} \left(\sum_{r=0}^{\nu-1} \frac{(-1)^{\nu-r} \nu!}{r!(\nu-r)!} (s_1^2 + s_2^2 + t_1^2 + t_2^2 - 2 - 2s_1s_2t_1t_2)^r \right. \\ & \quad \times [(s_1^2 - 1)(s_2^2 - 1)(1 - t_1^2)(1 - t_2^2)]^{\left(\frac{\nu-r}{2}\right)} \\ & \quad \times \left\{ \sum_{\lambda=0}^{\mu} \frac{(\nu-r)!}{\lambda!(\nu-r-\lambda)!} \sum_{i=0}^{\infty} F_{i,\nu-r-2\lambda} P_i^{\nu-r-2\lambda}(s \prec) \right. \\ & \quad \times Q_i^{\nu-r-2\lambda}(s \succ) P_i^{\nu-r-2\lambda}(t_1) P_i^{\nu-r-2\lambda}(t_2) \\ & \quad \left. + \frac{(\nu-r)!}{\left(\frac{\nu-r}{2}\right)!} \sum_{i=0}^{\infty} F_{i0} P_i(s \prec) Q_i(s \succ) P_i(t_1) P_i(t_2) \right\}, \end{aligned} \quad (\text{A.14})$$

where μ is defined by

$$\mu = \begin{cases} \frac{(\nu-r)}{2} - 1 & \text{for even } (\nu-r) \\ \frac{(\nu-r-1)}{2} & \text{for odd } (\nu-r) \end{cases} \quad (\text{A.15})$$

where the second term in the curly brackets exists only for even $(\nu-r)$. Now substituting (A.14) in the integral I_p , Eq. (37), and integrating over Φ_1 and Φ_2

gives

$$\begin{aligned}
 I_p(m, n, k, \ell, \delta, \eta) &= 4\pi^2 \left(\frac{1}{2}\right)^{2\nu-1} \left\{ \sum_{\kappa_1=0}^{\nu} \sum_{\kappa_2=0}^{\kappa_1} \sum_{\kappa_3=0}^{\kappa_2} \sum_{\kappa_4=0}^{\kappa_3} \sum_{\kappa_5=0}^{\kappa_4} \frac{(-2)^{\kappa_4} \nu!}{(\nu - \kappa_1)! \kappa_5!} \right. \\
 &\times \prod_{i=1}^4 \frac{1}{(\kappa_i - \kappa_{i+1})!} \sum_{\tau=0}^{\infty} F_{\tau 0} X_{\tau}^0(m + 2\nu - 2\kappa_1 + \kappa_5, n + 2\kappa_1 - 2\kappa_2 + \kappa_5, \\
 &\quad k + 2\kappa_2 - 2\kappa_3 + \kappa_5, \ell + 2\kappa_3 - 2\kappa_4 + \kappa_5, \delta, \eta) \\
 &+ \sum_{\epsilon_1=0}^{\nu-1} \sum_{\epsilon_2=0}^{\epsilon_1} \sum_{\epsilon_3=0}^{\epsilon_2} \sum_{\epsilon_4=0}^{\epsilon_3} \sum_{\epsilon_5=0}^{\epsilon_4} \sum_{\epsilon_6=0}^{\epsilon_5} \frac{(-2)^{\nu-\epsilon_1} \nu!}{\epsilon_6!} \left(\prod_{i=1}^5 \frac{1}{(\epsilon_i - \epsilon_{i+1})!} \right) \\
 &\times \left[\sum_{\varsigma=0}^{\mu} \frac{1}{\varsigma! (\nu - \epsilon_1 - \varsigma)!} \left(\prod_{j=1}^4 \sum_{\sigma_j=0}^{\varsigma} \frac{\varsigma!}{\sigma_j! (\varsigma - \sigma_j)!} \right) (-1)^{(2\varsigma - \sigma_1 - \sigma_2 + \sigma_3 + \sigma_4)} \right. \\
 &\times \sum_{\tau_1=0}^{\infty} F_{\tau_1; \nu - \epsilon_1 - 2\varsigma} X_{\tau_1}^{\nu - \epsilon_1 - 2\varsigma}(m + 2\nu - 2\epsilon_2 + \epsilon_6 + 2\sigma_1, \\
 &\quad n + 2\epsilon_2 - 2\epsilon_3 + \epsilon_6 + 2\sigma_2, k + 2\epsilon_3 - 2\epsilon_4 + \epsilon_6 + 2\sigma_3, \\
 &\quad \ell + 2\epsilon_4 - 2\epsilon_5 + \epsilon_6 + 2\sigma_4, \delta, \eta) \\
 &+ \frac{(\nu - \epsilon_1)!}{\left(\frac{\nu - \epsilon_1}{2}\right)!} \left(\prod_{r=0}^4 \sum_{\xi_r=0}^{(\nu - \epsilon_1)/2} \frac{\left(\frac{\nu - \epsilon_1}{2}\right)!}{\xi_r! \left(\frac{\nu - \epsilon_1}{2} - \xi_r\right)!} \right) (-1)^{\nu - \epsilon_1 - \xi_1 - \xi_2 + \xi_3 + \xi_4} \\
 &\times \sum_{\tau_2=0}^{\infty} F_{\tau_2 0} X_{\tau_2}^0(m + \nu - \epsilon_1 - 2\epsilon_2 + \epsilon_6 + 2\xi_1, n + 2\epsilon_2 - 2\epsilon_3 + \epsilon_6 + 2\xi_2, \\
 &\quad k + 2\epsilon_3 - 2\epsilon_4 + \epsilon_6 + 2\xi_3, \ell + 2\epsilon_4 - 2\epsilon_5 + \epsilon_6 + 2\xi_4, \delta, \eta) \left. \right\}. \quad (\text{A.16})
 \end{aligned}$$

Again, the last term exists only for $(\nu - \epsilon_1)$ is even, while the integral X_{τ}^{μ} is given by

$$\begin{aligned}
 X_{\tau}^{\mu}(m, n, k, \ell, \delta, \eta) &= \int s_1^m s_2^n e^{-\delta(s_1 + s_2)} P_{\tau}^{\mu}(s \prec) Q_{\tau}^{\mu}(s \succ) \\
 &\times W^{\mu} t_1^k P_{\tau}^{\mu}(t_1) t_2^{\ell} P_{\tau}^{\mu}(t_2) e^{\eta(t_1 - t_2)} ds_1 ds_2 dt_1 dt_2 \quad (\text{A.17})
 \end{aligned}$$

with

$$W^2 = (s_1^2 - 1) (s_2^2 - 1) (1 - t_1^2) (1 - t_2^2). \quad (\text{A.18})$$

The solution of the above integral can be written as

$$X_{\tau}^{\mu}(m, n, k, \ell, \delta, \eta) = Z_{\tau}^{\mu}(m, n, \delta) G_{\tau}^{\mu}(k, \eta) G_{\tau}^{\mu}(\ell, -\eta), \quad (\text{A.19})$$

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where

$$Z_{\tau}^{\mu}(m, n, \delta) = \int_1^{\infty} x_1^m x_2^n e^{-\delta(x_1+x_2)} (x_1^2-1)^{\mu/2} (x_2^2-1)^{\mu/2} \times P_{\tau}^{\mu}(x_1) Q_{\tau}^{\mu}(x_2) dx_1 dx_2 \quad (\text{A.20})$$

and

$$G_{\tau}^{\mu}(\lambda, \pm\eta) = \int_{-1}^1 (1-x^2)^{\mu/2} x^{\lambda} P_{\tau}^{\mu}(x) e^{\pm\eta x} dx. \quad (\text{A.21})$$

The solution of G_{τ}^{μ} is simple. Using [28]

$$P_{\tau}^{\mu}(x) = (1-x^2)^{\mu/2} \frac{d^{\mu} P_{\tau}(x)}{dx^{\mu}} \quad (\text{A.22})$$

and

$$P_{\tau}(x) = \sum_{\beta=0}^{\tau} p_{\tau}^{\beta} x^{\beta}. \quad (\text{A.23})$$

We get

$$G_{\tau}^{\mu}(\lambda, \pm\eta) = \sum_{\beta=\mu}^{\tau} \frac{\beta!}{(\beta-\mu)!} p_{\tau}^{\beta} \times \sum_{\zeta=0}^{\mu} (-1)^{\zeta} \frac{\mu!}{\zeta!(\mu-\zeta)!} B_{\lambda+\beta-\mu+2\zeta}(\pm\eta). \quad (\text{A.24})$$

The Z-integral, on the other hand, is written as

$$Z_{\tau}^{\mu}(m, n, \delta) = \int_1^{\infty} x_1^m (x_1^2-1)^{\mu/2} e^{-\delta x_1} Q_{\tau}^{\mu}(x_1) dx_1 \int_1^{x_1} x_2^n (x_2^2-1)^{\mu/2} e^{-\delta x_2} P_{\tau}^{\mu}(x_2) dx_2 + \int_1^{\infty} x_2^n (x_2^2-1)^{\mu/2} e^{-\delta x_2} Q_{\tau}^{\mu}(x_2) dx_2 \int_1^{x_2} x_1^m (x_1^2-1)^{\mu/2} e^{-\delta x_1} P_{\tau}^{\mu}(x_1) dx_1 = H_{\tau}^{\mu}(m, n, \delta) + H_{\tau}^{\mu}(n, m, \delta), \quad (\text{A.25})$$

where

$$H_{\tau}^{\mu}(m, n, \delta) = \int_1^{\infty} x^m (x^2-1)^{\mu/2} e^{-\delta x} Q_{\tau}^{\mu}(x) dx \times \int_1^x y^n (y^2-1)^{\mu/2} e^{-\delta y} P_{\tau}^{\mu}(y) dy. \quad (\text{A.26})$$

The y-integral is solved using the relations (A.22) and (A.23) to give

$$\sum_{v=0}^{\tau} \frac{v!}{(v-\mu)!} p_{\tau}^v \sum_{\rho=0}^{\mu} (-1)^{(3\mu-2\rho)/2} \frac{\mu!}{\rho!(\mu-\rho)!} A_{n+\beta-\mu+2\rho}(1, x, \delta), \quad (\text{A.27})$$

so that the H -integral will be given by

$$\begin{aligned} H_{\tau}^{\mu}(m, n, \delta) &= \sum_{v=0}^{\tau} \frac{v!}{(v-\mu)!} p_{\tau}^v \sum_{\rho=0}^{\mu} (-1)^{(3\mu-2\rho)/2} \frac{\mu!}{\rho!(\mu-\rho)!} \times \\ &\times \sum_{\kappa=0}^{n+\beta+2\rho-\mu} \frac{(n+\beta+2\rho-\mu)!}{(n+\beta+2\rho-\mu-\kappa)!} \left\{ \frac{e^{-\delta}}{\delta^{\kappa+1}} F_{\tau}^{\mu}(m, \delta) \right. \\ &\quad \left. - \frac{1}{\delta^{\kappa+1}} F_{\tau}^{\mu}(m+n+v+2\rho-\mu-\kappa, \delta) \right\}, \quad (\text{A.28}) \end{aligned}$$

where

$$F_{\tau}^{\mu}(\nu, \delta) = \int_1^{\infty} x^{\nu} (x^2 - 1)^{\mu/2} e^{-\delta x} Q_{\tau}^{\mu}(x) dx. \quad (\text{A.29})$$

The solution of this integral can be obtained through the recurrence relation

$$F_{\tau}^{\mu}(\nu, \delta) = (-1)^{\mu/2} [(\mu-\tau-1)F_{\tau}^{\mu-1}(\nu, \delta) + (\mu+\tau-1)F_{\tau-1}^{\mu-1}(\nu, \delta)], \quad (\text{A.30})$$

where

$$F_{\tau}^0(\nu, \delta) = F_{\tau}(\nu, \delta) = \int_1^{\infty} x^{\nu} e^{-\delta x} Q_{\tau}(x) dx. \quad (\text{A.31})$$

This is solved using the relation [28]

$$Q_{\xi}(x) = \frac{1}{2} P_{\xi}(x) \ln \left(\frac{x+1}{x-1} \right) + \sum_{\eta=0}^{\xi} q_{\xi}^{\eta} x^{\eta}, \quad (\text{A.32})$$

so that

$$\begin{aligned} F_{\tau}(\nu, \delta) &= \frac{1}{2} \sum_{\rho=0}^{\tau} p_{\tau}^{\rho} \lim_{\epsilon \rightarrow 0} \int_{1+\epsilon}^{\infty} x^{\nu+\rho} \ln \left(\frac{x+1}{x-1} \right) e^{-\delta x} dx \\ &\quad + \sum_{\eta=0}^{\tau} q_{\tau}^{\eta} \int_1^{\infty} x^{\nu+\eta} e^{-\delta x} dx \\ &= \frac{1}{2} \sum_{\rho=0}^{\tau} p_{\tau}^{\rho} F_0(\nu+\rho, \delta) + \sum_{\eta=0}^{\tau} q_{\tau}^{\eta} A_{\nu+\eta}(1, \delta), \quad (\text{A.33}) \end{aligned}$$

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where the integral

$$F_0(\lambda, \delta) = \lim_{\epsilon \rightarrow 0} \int_{1+\epsilon}^{\infty} x^\lambda \ln\left(\frac{x+1}{x-1}\right) e^{-\delta x} dx \quad (\text{A.34})$$

is solved through integration by parts to give

$$\begin{aligned} F_0(\lambda, \delta) = & \lim_{\epsilon \rightarrow 0} \sum_{\kappa=0}^{\lambda} \frac{\lambda!}{(\lambda-\kappa)!} \frac{1}{\delta^{\kappa+1}} \left\{ (1+\epsilon)^{\lambda-\kappa} e^{-\delta(1+\epsilon)} [\ln(2+\epsilon) - \ln \epsilon] \right. \\ & + (-1)^{\lambda-\kappa-1} e^{\delta} E_i(-2\delta - \epsilon\delta) + e^{-\delta} E_i(-\epsilon\delta) \\ & \left. + \sum_{\iota=1}^{\lambda-\kappa} \binom{\lambda-\kappa}{\iota} [(-1)^{\lambda-\kappa-\iota} e^{\delta} A_{\iota-1}(2+\epsilon, \delta) - e^{-\delta} A_{\iota-1}(\epsilon, \delta)] \right\}, \quad (\text{A.35}) \end{aligned}$$

where $E_i(x)$ is the logarithmic integral. Now using (A.5) and passing to the limit we get

$$\begin{aligned} F_0(\lambda, \delta) = & \ln(2\delta + C) A_\lambda(1, \delta) - E_i(-2\delta) A_\lambda(-1, \delta) \\ & + \frac{e^{-\delta}}{\delta} \sum_{\nu=0}^{\lambda} \frac{\lambda!}{\delta^\nu} \left\{ \sum_{\iota=1}^{\lambda-\nu} \frac{1}{\iota! (\lambda-\nu-\iota)!} \right. \\ & \left. \times \left[(-1)^{\lambda-\nu-\iota} \sum_{\varsigma=0}^{\iota-1} \frac{(\iota-1)!}{\iota-\varsigma-1} \frac{2^{\iota-\varsigma-1}}{\delta^{\varsigma+1}} - \frac{(\iota-1)!}{\delta^\iota} \right] \right\}, \quad (\text{A.36}) \end{aligned}$$

where $C = 0.57721566490153286060651209008240$, is the Euler constant.

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