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Alejandro Ferrón
Universidad Nacional de Córdoba

Pablo Serra
Universidad Nacional de Córdoba

Sabre Kais
Birck Nanotechnology Center and Department of Chemistry, Purdue University, kais@purdue.edu

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Stability conditions for hydrogen-antihydrogen–like quasimolecules

Alejandro Ferrón* and Pablo Serra†
Facultad de Matemática, Astronomía y Física, Universidad Nacional de Córdoba and IFFAMAF (CONICET), Ciudad Universitaria, 5000 Córdoba, Argentina

Sabre Kais‡
Department of Chemistry and Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana 47907, USA

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We present a detailed study of the stability conditions of hydrogen-antihydrogen–like quasimolecules using both variational and finite-size-scale calculations. The stability diagram of the nuclear charge \( Z \) as a function of the internuclear distance \( R \) shows bound and unbound regions separated by a first-order critical line. Calculations of the leptonic annihilation rate show a peculiar behavior for nuclear charges \( Z \geq 2 \), which was not observed for the hydrogen-antihydrogen quasimolecule; it goes through a maximum before it decays exponentially for large interhadronic distances. This might have a practical impact on the study of stability of matter-antimatter systems.

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I. INTRODUCTION

The behavior and properties of antimatter have been the subject of research for many decades [1,2]. However, recent experimental success in the production of antihydrogen atoms and the potential application of antihydrogen for charge-parity-time invariance and the weak equivalence principle have raised interest in the interaction between atoms and antimat\( \text{o} \)s [3–5]. Froelich et al. have found that, when colliding at low speeds, hydrogen and antihydrogen have a tendency to recombine into protonium (proton plus antiproton, \( \text{Pn} \)) and positronium (electron plus positron, \( \text{Ps} \)) before the particles and antiparticles annihilate. Both \( \text{Pn} \) and \( \text{Ps} \) are highly unstable but are slightly longer lived than they would be in the absence of the other pairing; that is, the positronium helps to screen the proton-antiproton interaction [6]. They also have shown that leptonic annihilation is three orders of magnitude slower than proton-antiproton annihilation [7].

In this work, we have calculated the complete stability diagram for hydrogen-antihydrogen–like molecules with varying nuclear charges to include the isoelectronic atoms of hydrogen such as \( \text{He}^+, \text{Li}^{2+}, \text{etc.} \), and their antimat\( \text{o} \)s. We also have shown that the leptonic annihilation rate has a peculiar behavior for nuclear charges \( Z \geq 2 \), which was not observed for the hydrogen-antihydrogen molecule; it goes through a maximum before it decays exponentially for large interhadronic distances. This might have a practical impact on the study of stability of matter-antimatter systems by preparing antihydrogenlike atoms.

The paper is organized as follows. In Sec. II, we briefly describe the hydrogen-antihydrogen like molecule. In Sec. III we present numerical and analytical results. Finally, the conclusions are given in Sec. IV.

II. MODEL

The hydrogen-antihydrogen–like molecules consists of four particles, two hadrons (a proton with a charge \( Z \) and an antiproton with a charge \( -Z \)) and two leptons (an electron and a positron). The leptonic Hamiltonian for a molecule formed with a one-electron atom with nuclear charge \( Z \geq 0 \) and a one-positron antimat\( \text{o} \) of nuclear charge \( -Z \), in the Born-Oppenheimer approximation, can be written as the Hamiltonian of an electron-positron pair in a finite dipole field of charges \( Z \) and \( -Z \) separated by a distance \( R \). In atomic units the Hamiltonian is given by

\[
H = h(Z,R;\tilde{r}_e) + h(-Z,R;\tilde{r}_p) - \frac{1}{r_{12}},
\]

where \( \tilde{r}_e \) and \( \tilde{r}_p \) denote the coordinates of the electron and the positron, respectively, \( r_{12} \) is the interelectronic distance, and \( h(Z,R;\tilde{r}) \) is the one-electron dipole Hamiltonian

\[
h(Z,R;\tilde{r}) = \frac{1}{2} \nabla^2 Z - \frac{1}{|\tilde{r} - \tilde{R}/2|} - \frac{1}{|\tilde{r} + \tilde{R}/2|},
\]

where the nuclei with charges \( Z \) and \( -Z \) \((Z>0)\) corresponding to the nuclei of the atom and the antimat\( \text{o} \) are located along the \( z \) axis at \( \frac{R}{2} \) and \( -\frac{R}{2} \), respectively.

In the separated-atom limit the ground state is given by a hydrogenlike atom and an antihydrogenlike atom. The corresponding energy is that of two noninteracting hydrogenlike atoms, \(-Z^2 \) a.u. In the opposite limit, the united-atom limit, the charges of the proton \((Z)\) and antiproton \((-Z)\) cancel each other, and thus the energy is that of an electron-positron pair, the ground state of the positronium atom, \(-\frac{Z^2}{R} \) a.u. The hadronic energy \(-\frac{Z^2}{R} \) is in this approximation an additive constant, and we are not taking it into account in our analysis.

III. GROUND-STATE STABILITY

In this section we study the ground-state stability of hydrogen-antihydrogen–like molecules against ionization...
and annihilation of the electron-positron pair. Numerical and analytical results are presented.

By variational arguments, using a product of two one-electron dipole wave functions \( \Phi_0 \) as a trial function, \( \Phi(r_e, \bar{r}_{e^*}) = \Phi_0(-\bar{r}_{e^*}) \Phi_0(r_e) \), we can show that the one-electron dipole (OED) is never the threshold system, 

\[
E_{0}(Z,R) \leq \langle \Phi | \hat{H} | \Phi \rangle = 2E_{\text{OED}}(Z,R) - \left\langle \Phi \left| \frac{1}{r_{12}} \right| \Phi \right\rangle < E_{\text{OED}}(Z,R). 
\]

The threshold system is an unbound electron-positron atom; therefore the threshold energy is \( \varepsilon_{\text{th}} = -\frac{1}{4} \) a.u. Thus, we have an upper bound for the stability line; the atom-antiatom system is stable if

\[
E_{\text{OED}}(Z,R) < \varepsilon_{\text{th}} = -\frac{1}{4},
\]

where \( E_{\text{OED}}(Z,R) \) is the energy of a one-electron dipole. Note that, because of matter-antimatter symmetry, \( E_{\text{OED}}(Z,R) = E_{\text{OED}}(Z,R) \), where \( E_{\text{OED}}(Z,R) \) is the energy of a one-positron dipole.

In order to apply the variational approach we used the trial wave function

\[
\Psi(r_{e^-}, \bar{r}_{e^+}) = \sum_{\{n\}} a_n \Phi_n(r_{e^-}, \bar{r}_{e^+}),
\]

where \( \{n\} \) represents the corresponding set of quantum numbers. The basis set \( \{\Phi_n\} \) is obtained using explicitly correlated James-Coolidge [8] type basis functions. In order to approximate the different quantities, we have to truncate the series Eq. (5) at order \( N \), where \( N \) is an integer number related to the powers in the James-Coolidge functions [8,9]. Then the Hamiltonian is replaced by an \( \bar{M}(N) \times \bar{M}(N) \) matrix, with \( M(N) \) being the number of elements in the truncated basis set at order \( N \). Using the Ritz variational method [10] we can evaluate an upper bound of the ground-state energy \( E_{0}(Z,R) \) of the Hamiltonian (1) and the corresponding coefficients \( a_n \) needed for the evaluation of the ground-state wave function. The critical line \( Z_c(R) \) for stability can be obtained by equating the ground-state energy, obtained from the variational calculation, to the threshold energy (\( \varepsilon_{\text{th}} = -1/4 \)),

\[
E_{0}(Z,R) - \varepsilon_{\text{th}} = 0.
\]

Finite-size scaling provides an alternative approach to evaluate critical parameters and critical exponents [11–13]. The critical exponent \( \alpha \) characterizes the near-threshold behavior of the energy and is given by

\[
E_{0}(Z,R) - \varepsilon_{\text{th}} \sim (Z - Z_c)^\alpha \quad \text{for } Z \rightarrow Z_c^+.
\]

This method has been developed for studying critical conditions in quantum mechanics [14–17]. In this approach, finite size relates to the number of elements in a basis set used to expand the exact wave function of a given Hamiltonian. Briefly, the critical line \( Z_c(R) \) and the critical exponent can be obtained from extrapolated values of the pseudocritical points \( Z_c^{(N)}(R) \) and pseudocritical exponents \( \alpha^{(N)} \), obtained from the finite-size scaling equation [15]:

\[
\Gamma(Z(R)) = Z_c^{(N)}; N - 1, N = \Gamma(Z(R)) = Z_c^{(N)}; N, N + 1 = \alpha^{(N)},
\]

where

\[
\Gamma(Z(R), N, N') = \frac{\Delta_N}{\Delta_{N} - \Delta_{N'}} = \frac{\ln(I_{Z_c^{(N)}(Z(R))}^{(N')})}{\ln(N'/N)},
\]

and \( I_{Z(R)} \) is the ionization energy \( E_{0} - \varepsilon_{\text{th}} \).

The integrals needed for the evaluation of the matrix elements required for the calculation of the ground-state energy and any other expectation value were obtained in a previous work [18] and used successfully in the study of the stability of two-electron diatomic molecules [9,19]. The finite-size-scaling approach has been successfully applied to calculate the critical parameters for few-electron systems [9,19–27].

In Fig. 1 we show the stability diagram for the ground-state energy of the hydrogen-antihydrogen–like quasimolecule calculated with the variational method (solid line) and the finite-size-scaling approach (dots); the two are in complete agreement. We also included in the diagram the one-electron (-positron) dipole threshold curve \( E_{\text{OED}}(Z,R) = 0 \) and the upper-bound curve obtained from the equation \( E_{\text{OED}}(Z,R) = -1/4 \). Note that the one-electron dipole threshold curve, which is a lower bound, is very close to the variational curve for large values of \( Z \geq 3 \), which shows that our calculations are accurate and reliable for large values of \( Z \). This is very important for a later analysis of the peculiar leptonic coalescence probability distribution. The possibility of binding two leptons in the case \( Z = 1 \) has been studied by many authors. The critical distance \( R_c(Z = 1) \) for this particular system can be calculated with our method as in Fig. 1, obtaining \( R_c^{2052} = 0.7745 \) from the variational calculation.

FIG. 1. Ground-state stability diagram for one-electron–one-positron atom-antiatom molecules in atomic units. The solid line represents the variational calculations and the dots are the finite-size-scaling calculations. The dotted line is obtained from the one-electron dipole threshold and the dashed line from the one-electron dipole upper-bound condition.
The stability conditions for hydrogenic atoms are given by

\[ E(Z) = \frac{Z^2}{R^2} + O(R), \quad R \to \infty, \quad Z \geq Z_c(R). \]  

(13)

Equations (11) and (13) show that \( P(Z; R) \) presents a discontinuity at \( Z=Z_c(R) \), at least for large values of \( R \).

The critical exponent \( \alpha \) can be calculated analytically for large values of \( R \), using the unperturbed wave function Eq. (12) to obtain the energy up to second order. The Hamiltonian could be written as the sum of three terms, a hydrogen-like atom, an antihydrogen-like atom, and a perturbation potential \( V \), the interaction between matter and antimatter:

\[ H = h_0(p, e^-) + h_0(\bar{p}, e^+) + V, \]  

(14)

where

\[ V = \frac{Z}{|R - \vec{r}|} + \frac{Z}{|R + \vec{r}|} - \frac{1}{|R + \vec{r} - \vec{r}_e|}. \]  

(15)

Here \( \vec{R} \) is the vector from the antinuclei to the nuclei, \( \vec{r}_e \) is the position of the electron with respect to the nuclei, and \( \vec{r}_+ \) is the position of the positron with respect to the antinuclei. A Taylor expansion in the variables \( \vec{r}_e/R, \vec{r}_+/R \) gives

\[ V = \frac{1}{R} \left[ 2Z - 1 + \frac{Z}{R} (z_e - z_+e^+) \right] + O(1/R^3). \]  

(16)

The first term, a monopole-monopole interaction, gives a first-order contribution \( E_0(1)=(2Z-1)/R \). All other terms in the complete expansion of \( V \) gave no first-order contribution. The second term, corresponding to the monopole-dipole interaction, gives

\[ E_0(2) = -C \frac{(1-Z)^2}{Z^2 R^4}, \]  

(17)

where \( C \) is a positive constant. For large values of \( R \),

\[ E_0 = -Z^2 \frac{2(Z-1/2)}{R} - C \frac{(1-Z)^2}{Z^2 R^4} + O(1/R^5). \]  

(18)

This expression shows that the energy at \( Z=1/2 \) is still less than the threshold energy for large (but finite) values of \( R \); then the critical charge is smaller than 1/2. Since \( Z_c \to 1/2 \) for \( R \to \infty \), then we can assume the form

\[ Z_c = 1 - \frac{\Delta}{2 R^\beta} \quad \text{for} \quad R \to \infty \]  

(19)

with \( \Delta \) and \( \beta \) positive constants. Thus expression in Eq. (18) gives

\[ \beta = 4, \quad \Delta = 4C. \]  

(20)

Using the standard definition for the critical exponent \( \alpha \) for the energy Eq. (7), we can obtain its value by studying the behavior of \( E_0-E_{th} \) for a charge close to but larger than \( Z_c \),

\[ E_0(Z,R) - E_{th} \simeq [-1 + O(1/R)](Z - Z_c) \quad \text{for} \quad R \to \infty. \]  

(21)

This linear near-threshold behavior gives \( \alpha=1 \) for large values of \( R \). The critical exponent is also \( \alpha=1 \) for two-electron

\[ P(Z; R) \sim e^{-2ZR} \left( \frac{Z^2 R^2}{6} + O(R) \right), \quad R \to \infty, \quad Z \geq Z_c(R). \]  

(13)

This linear near-threshold behavior gives \( \alpha=1 \) for large values of \( R \).
systems, like the heliumlike atom [14] and the H$_2$ molecule [19]. Thus, we assume that the critical exponent is $\alpha=1$ for the whole critical line. This value of the exponent implies that above the critical line defined by the condition $E_0(Z_c, R) = -1/4$ [17], the molecule is bound, having the same energy as for the electron-positron pair.

In Fig. 2 we show the leptonic annihilation probability distribution as a function of $R$ for three different values of $Z$. For $Z=1$, we reproduced the earlier known results [31]. For $Z=2$, the probability shows a maximum near the critical radius $R_c$, which is absent in the case of the neutral H-H molecule [31]. For $Z=3$, the Li$^{2+}$-Li$^{2+}$ molecule, the probability density presents a notable maximum at $R=2.1R_c$. In Fig. 3 the electron-positron average distance $\langle r_{12} \rangle$ is plotted as a function of $R$ for $Z=0.8,1.2,3$. These calculations were done with 679 basis functions. It is interesting to note that for large values of $Z$ there exists a minimum in the interparticle distance. This minimum disappears for $Z=0.8$ while for $Z=1$ it starts to be distinguishable. Finally, in Fig. 4 we plot contours of the ground-state leptonic density for $Z=1$ and 3 for fixed interhadronic separation $R=2R_c$ in the $(x/R, z/R)$ plane, where the hadronic axis points along the $z$ axis. Due to the special symmetry, only the electronic density is shown [28]. While for the hydrogen-antihydrogen molecule ($Z=1$), the shown leptonic density is almost identical to that of an isolated hydrogen atom, a deviation from the spherical symmetry is apparent for $Z=3$ (Li$^{2+}$-Li$^{2+}$ molecule) for the same values of $R/R_c$. The density contours are consistent with the results shown in previous figures; the large overlap for $Z=3$ is responsible for the maximum in the leptonic annihilation probability distribution.

**IV. CONCLUSION**

Our results for the hydrogen-antihydrogen quasimolecule ($Z=1$) are in complete agreement with the known results [31]. The physical picture is clear for large values of $R$: for a fixed value of $Z$ there exists a value of $R$ ($R^*$) such that the overlap between the leptons is essentially zero. We can get a crude estimation of the value of $R^*$. For an isolated one-electron atom (or antiatom) the probability to find an electron at a distance $r=r_i$ from the nucleus, where $r_i=\langle r \rangle+\Delta r$ and $\Delta r=\sqrt{\langle r^2 \rangle-\langle r \rangle^2}$, is $P(r_i) = 4\pi r^2_0 |\psi|^2 dr$ for all values of $Z$. Thus, defining $R^*$ as the distance between hadrons such that the overlap between leptons is essentially zero, $R^*(Z)=2r_i(Z)$, we get $ZR^*(Z) = 3(1+\sqrt{2}) \approx 7.2$.

For small values of $R$ we have a different picture. For large values of $R$ the leptonic density is almost identical to that of an isolated atom; as we decrease the interhadronic distance, for any value of the nuclear charge, a deviation from the spherical symmetry appears. For small values of the nuclear charge the behavior of the system is qualitatively similar to that of the known hydrogen-antihydrogen quasimolecule [28,30,31]. The most interesting results appear for large values of $Z$ and small values of $R$. The critical line $Z_c(R)$ goes asymptotically to the one-electron dipole critical line for large values of $Z$ as seen in Fig. 1. As we see in Fig. 3 for $Z=2$ and 3, the mean value of the interleptonic distance has a minimum for $R=1$ and $R=0.7$, respectively. Close to the minimum the overlap between the electron density and the positron density increases with $Z$ as shown in Fig. 4, giving a maximum in $P(Z,R)$. The leptons are not around one nucleus, but surrounding both hadrons. Thus the nuclear potential could be approximated by a dipolar field near the critical moment. Therefore the leptons are weakly bound to the nuclei and the wave function goes to a quasispherical ground state close to the free leptonic wave function, but with the center of mass weakly bound by the dipole field.

The stability conditions of exotic hydrogen-antihydrogen–like quasimolecules have been discussed using variational and finite-size-scaling calculations. Calculations of the leptonic annihilation rate shows a maximum for nuclear charges $Z=2$ which was not observed for the hydrogen-antihydrogen quasimolecule. In view of the ongoing antihydrogen experiments, studies of antihydrogenlike atoms might have a practical impact on the study of stability of matter-antimatter systems.

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