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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 scaling 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 antiatoms [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, Pn) and positronium (electron plus positron, Ps) before the particles and antiparticles annihilate. Both Pn and 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 He^+ , Li^{2+} , etc., and their antiatoms. 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 $Z > 0$ and a one-positron antiatom 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

$$\mathcal{H} = h(Z, R; \vec{r}_{e^-}) + h(-Z, R; \vec{r}_{e^+}) - \frac{1}{r_{12}}, \quad (1)$$

where \vec{r}_{e^-} and \vec{r}_{e^+} denote the coordinates of the electron and the positron, respectively, r_{12} is the interleptonic distance, and $h(Z, R; \vec{r})$ is the one-electron dipole Hamiltonian

$$h(Z, R; \vec{r}) = -\frac{1}{2} \nabla^2 - Z \left(\frac{1}{|\vec{r} - \vec{R}/2|} - \frac{1}{|\vec{r} + \vec{R}/2|} \right), \quad (2)$$

where the nuclei with charges Z and $-Z$ ($Z > 0$) corresponding to the nuclei of the atom and the antiatom 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, $-\frac{1}{4}$ 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

*ferron@tero.fis.uncor.edu

†serra@famaf.unc.edu.ar

‡kais@purdue.edu

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 ϕ_0 as a trial function, $\Phi(\vec{r}_{e^+}, \vec{r}_{e^-}) = \phi_0(-\vec{r}_{e^+})\phi_0(\vec{r}_{e^-})$, we can show that the one-electron dipole (OED) is never the threshold system,

$$E_0(Z, R) \leq \langle \Phi | \mathcal{H} | \Phi \rangle = 2E_{\text{OED}}(Z, R) - \left\langle \Phi \left| \frac{1}{r_{12}} \right| \Phi \right\rangle < E_{\text{OED}}(Z, R). \quad (3)$$

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

$$E_{\text{OED}}(Z, R) < \mathcal{E}_{\text{th}} = -\frac{1}{4}, \quad (4)$$

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

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

$$\Psi(\vec{r}_{e^-}, \vec{r}_{e^+}) = \sum_{\{n\}} a_n \Phi_n(\vec{r}_{e^-}, \vec{r}_{e^+}), \quad (5)$$

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 $M(N) \times M(N)$ 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 $E_0^{(N)}(Z, R)$ of the Hamiltonian (1) and the corresponding coefficients $a_n^{(N)}$ 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 ($\mathcal{E}_{\text{th}} = -1/4$),

$$[E_0^{(N)}(Z, R) - \mathcal{E}_{\text{th}}]_{Z=Z_c^{(N)}} = 0. \quad (6)$$

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

$$E_0(Z, R) - \mathcal{E}_{\text{th}} \sim (Z - Z_c)^{\alpha} \quad \text{for } Z \rightarrow Z_c^+. \quad (7)$$

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

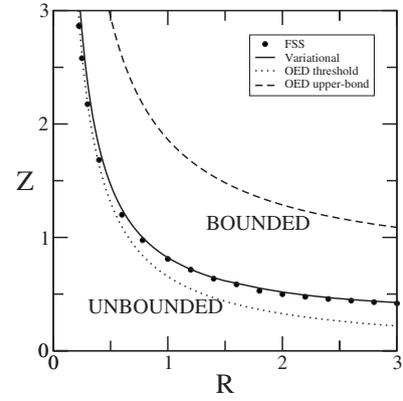


FIG. 1. Ground-state stability diagram for one-electron-one-positron atom-antiatom molecules in atomic units. The solid line represents the variational calculations and the dots are the finite-size-scaling calculations. The dotted line is obtained from the one-electron dipole threshold and the dashed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

points $Z_c^{(N)}(R)$ and pseudocritical exponents $\alpha^{(N)}$, obtained from the finite-size scaling equation [15]:

$$\Gamma(Z(R) = Z_c^{(N)}; N-1, N) = \Gamma(Z(R) = Z_c^{(N)}; N, N+1) = \alpha^{(N)}, \quad (8)$$

where

$$\Gamma(Z(R); N, N') = \frac{\Delta_{\mathcal{H}}}{\Delta_{\mathcal{H}} - \Delta_{\partial \mathcal{H} / \partial Z}}, \quad (9)$$

$$\Delta_{\mathcal{H}}(Z(R); N, N') = \frac{\ln(I_{Z(R)}^{(N)} / I_{Z(R)}^{(N')})}{\ln(N'/N)},$$

and $I_{Z(R)}$ is the ionization energy $I_{Z(R)} \equiv E_0 - \mathcal{E}_{\text{th}}$.

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 $Z \sim 3$, 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 $R_c^{\text{var}} = 0.7745$ from the variational calculation,

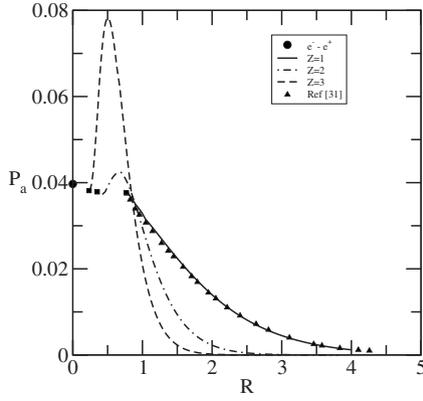


FIG. 2. Leptonic annihilation probability distribution as a function of $R > R_c$ (a.u.) (R_c black square) for three different values of Z (a.u.). For the H-H molecule P decreases monotonically with increasing R , but for the $\text{He}^+\text{-He}^+$ and $\text{Li}^{2+}\text{-Li}^{2+}$ molecules the probabilities reach a maximum for stable configurations before decreasing with increasing R .

$R_c^{\text{FSS}} = 0.7599$ from finite-size-scaling (FSS) calculations, $R_c^{\text{UB}} = 3.855$ from the upper-bound line, and $R_c^{\text{LB}} = 0.655$ from the lower-bound line. The variational and FSS results are in agreement with recent calculations [29,28].

The conditional probability density $P(R)$ for the electron and positron to coalesce while the hadrons are at a distance R apart is given by [7]

$$P(Z;R) = \langle \delta(\vec{r}_{e^-} - \vec{r}_{e^+}) \rangle = \int d^3x_{e^-} \int d^3x_{e^+} |\Psi_0(Z,R;\vec{r}_{e^-},\vec{r}_{e^+})|^2 \delta(\vec{r}_{e^-} - \vec{r}_{e^+}). \quad (10)$$

For the unbound electron-positron pair, this probability does not depend on the hadronic parameters R and Z and is given by

$$P(Z;R < R_c(Z)) = |\psi_0(0)|^2 = 1/(8\pi), \quad (11)$$

where $\psi_0(\vec{r})$ is the ground-state wave function of the hydrogenic atom with reduced mass $\mu=1/2$.

For $R \rightarrow \infty$, the interaction between the atom and the antiatom can be neglected; the total energy is the sum of two hydrogenlike atomic energies $E_0(Z,R=\infty) = -Z^2$. Then the system turns metastable at $Z^* = 1/2$, where the energy is degenerate with the energy of the unbound electron-positron pair. The metastable region $Z < Z^* = 1/2$ might correspond to long-lived resonances in the exact four-body solution of the problem.

For large values of R , the ground-state wave function can be approximated by the product of hydrogenic functions centered at the hadronic positions,

$$\Psi_0(Z,R \rightarrow \infty; \vec{r}_{e^-}, \vec{r}_{e^+}) \simeq \psi_0(\vec{r}_{e^-} - \vec{R}/2) \psi_0(\vec{r}_{e^+} + \vec{R}/2). \quad (12)$$

In this approximation, $P(Z;R)$ can be calculated analytically:

$$P(Z;R) \sim e^{-2ZR} \left(\frac{Z^2 R^2}{6} + O(R) \right), \quad R \rightarrow \infty, \quad Z \geq Z_c(R). \quad (13)$$

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 α 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 hydrogenlike atom, an antihydrogenlike atom, and a perturbation potential V , the interaction between matter and antimatter:

$$H = h_0(p, e^-) + h_0(\bar{p}, e^+) + V, \quad (14)$$

where

$$V = \frac{Z}{|\vec{R} - \vec{r}_+|} + \frac{Z}{|\vec{R} + \vec{r}_-|} - \frac{1}{|\vec{R} + \vec{r}_- - \vec{r}_+|}. \quad (15)$$

Here \vec{R} is the vector from the antinuclei to the nuclei, \vec{r}_- 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 $\vec{r}_-/R, \vec{r}_+/R$ gives

$$V = \frac{1}{R} \left(2Z - 1 + \frac{1-Z}{R} (z_- - z_+) \right) + O(1/R^3). \quad (16)$$

The first term, a monopole-monopole interaction, gives a first-order perturbation 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

$$E_0^{(2)} = -\mathcal{C} \frac{(1-Z)^2}{Z^4 R^4}, \quad (17)$$

where \mathcal{C} is a positive constant. For large values of R ,

$$E_0 = -Z^2 + \frac{2(Z-1/2)}{R} - \mathcal{C} \frac{(1-Z)^2}{Z^4 R^4} + O(1/R^5). \quad (18)$$

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 $Z_c \rightarrow 1/2$ for $R \rightarrow \infty$, then we can assume the form

$$Z_c = \frac{1}{2} - \frac{\Delta}{R^\beta} \quad \text{for } R \rightarrow \infty \quad (19)$$

with Δ and β positive constants. Thus expression in Eq. (18) gives

$$\beta = 4, \quad \Delta = 4\mathcal{C}. \quad (20)$$

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

$$E_0(Z,R) - \mathcal{E}_{\text{th}} \sim [-1 + O(1/R)](Z - Z_c) \quad \text{for } R \rightarrow \infty. \quad (21)$$

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

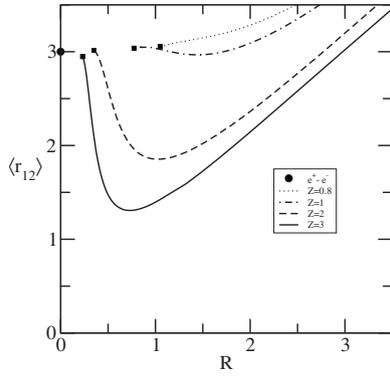


FIG. 3. Average distance $\langle r_{12} \rangle$ (a.u.) between leptons as a function of $R > R_c$ (a.u.) (R_c black square) for different values of $Z = 0.8, 1, 2, 3$ a.u.

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 $E_0(Z_c(R), R) = -1/4$ [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 $R \approx 2.1R_c$. 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

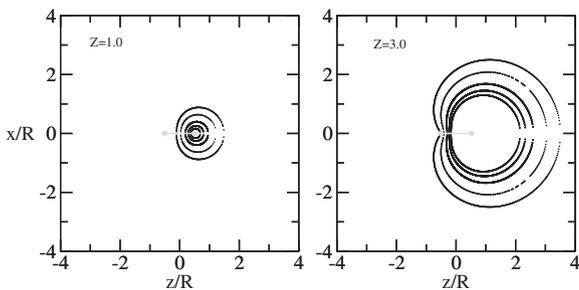


FIG. 4. Contours of leptonic densities in the ground state for $Z=1$ and 3 a.u. molecules for fixed interhadronic separation $R=2R_c$ (a.u.).

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 $r \leq r_t$ from the nucleus, where $r_t(Z) = \langle r \rangle + \Delta r$ and $\Delta r = \sqrt{\langle r^2 \rangle - \langle r \rangle^2}$, is $P(r_t) = 4\pi \int_0^{r_t} |\psi|^2 r^2 dr \sim 0.975$ for all values of Z . Thus, defining R^* as the distance between hadrons such that the overlap between leptons is essentially zero, $R^*(Z) = 2r_t(Z)$, we get $ZR^*(Z) = 3(1 + \sqrt{2}) \sim 7.2$.

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 $R \approx 1$ and $R \approx 0.7$, 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 $Z \geq 2$ 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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