Proof that the Hydrogen-Antihydrogen Molecule Is Unstable

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In the framework of nonrelativistic quantum mechanics we derive a necessary condition for four Coulomb charges $(m_1^+, m_2^-, m_3^+, m_4^-)$, where all masses are assumed finite, to form the stable system. The obtained stability condition is physical and is expressed through the required minimal ratio of Jacobi masses. In particular, this provides the rigorous proof that hydrogen-antihydrogen and muonium-antimuonium molecules and hydrogen-positron-muon systems are unstable. It also proves that replacing hydrogen in the hydrogen-antihydrogen molecule with its heavier isotopes does not make the molecule stable. These are the first rigorous results on the instability of these systems.

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Introduction.—Recent success in the production of trapped antihydrogen atoms [1] has renewed interest in the interaction of matter with antimatter and especially in the hydrogen-antihydrogen system (H-$\bar{\text{H}}$). The system of hydrogen and antihydrogen is known to decay into protonium ($p\bar{p}$) and positronium (e^+e^-); the estimated lifetimes of such fragmentation are presented in [2]. It has long been conjectured that with pure Coulomb forces no bound state of hydrogen-antihydrogen exists. The numerical evidence supports this conjecture [3], yet there is a lack of rigorous proof as remarked by some authors [4–6]. Our aim in this Letter is (i) to supply such a proof under the assumption that only Coulomb forces act between the constituents and (ii) to provide insight into the screening effect within the system of four charged particles. From our results it also follows that the systems $p\mu^-e^+e^-$, $\mu^+\mu^-e^+e^-$, $d\bar{p}e^+e^-$, $t\bar{p}e^+e^-$ (d, t stand for deutron and tritium) are unstable. These are new results. Let us remark that taking strong interactions into account, which are present in the hydrogen-antihydrogen system, would hardly make this molecule stable because of the proton-antiproton annihilation.

To avoid any confusion we would like to stress that under *instability* we understand the absence of bound states below the dissociation thresholds; otherwise the system is called *stable*; the same definition is used in [3–10]. We do not consider such issues as long-living resonances or bound states embedded into the continuum. The stability problem for particles interacting through Coulomb forces is complicated even when the number of particles is three or four. Direct variational calculations are helpful but they can only prove that a system is stable but no definitive conclusion about the instability can be drawn, since any enrichment of basis functions lowers the binding energies. Thirring, in his book [7], has placed the stability problem for three unit Coulomb charges as number one on the list of difficult unsolved problems. Since that time, a lot of light has been shed on stability of these three-body systems; the stability domain has been outlined partly by semianalytical methods as in [8] and partly by analytical ones as in [7,9,10] ([9] gives an excellent review of these matters). Yet not much has been known about four-body systems; the stability domain for masses was tentatively sketched in [5] (see also [6]) and from the present rigorous analysis appears to be correct.

The physical reason for instability of H-$\bar{\text{H}}$ is the screening effect. In [10] we have shown that the screening effect in the system of three charged particles can be expressed through the critical ratio of Jacobi masses. These masses are inverse proportional to the Bohr radii of two orbits, the orbit within the pair of particles (the pair that sets up the dissociation threshold), and the orbit of the third particle in the field of this pair with respect to the pair's center of mass. If the orbit of the third particle has a much larger radius, the attractive force acting on it is screened and the system must be unbound.

The system of four unit charges $(m_1^+, m_2^-, m_3^+, m_4^-)$ can be unstable only against dissociation into two neutral pairs. Indeed, if the lowest dissociation threshold would be dissociation into one particle and the bound cluster of three particles, then these two objects would have opposite charges and the long-tailed Coulomb attraction between them would guarantee the existence of a bound state below the dissociation threshold. (Just the same argument explains why atoms are stable.) This suggests that we have to consider three orbits, two inner orbits of the neutral pairs, and the third orbit of the relative motion of these pairs. The Jacobi masses for the neutral pairs are $\mu_x = m_1^+m_2^-/(m_1^+ + m_2^-)$ and $\mu_y = m_3^+m_4^-/(m_3^+ + m_4^-)$. The Jacobi mass corresponding to the relative motion of these two pairs is $\mu_R = (m_1^+ + m_2^-)(m_3^+ + m_4^-)/(m_1^+ + m_2^- + m_3^+ + m_4^-)$. Pay attention that we order the particles so that among two possible rearrangements into neutral pairs the lowest energy threshold corresponds to the dissociation into $(m_1^+m_2^-) + (m_3^+m_4^-)$ and the pairs are ordered so that $\mu_x \geq \mu_y$. It is easy to check that $\mu_R \geq 4\mu_y$ if the particles are ordered as above.

Let us consider the screening effect within the system of four particles keeping in mind that the Bohr radii of the orbits are inverse proportional to the Jacobi masses. The condition $\mu_y \ll \mu_R$ alone is not sufficient for the screening effect to take over. For example, Bressanini *et al.* [3] have collected the convincing evidence that the system $(m_1^+, 1^-, m_3^+, 1^-)$ is stable for any m_1^+ and m_3^+. The three-body system $(m_1^+, 1^-, 1^-)$ is always stable and if $m_3^+ \ll 1$ we run into the situation, where $\mu_y \ll \mu_R$ and $\mu_R \approx \mu_x$, and still the whole system is stable. When $\mu_R \ll \mu_x$, it is right to expect screening, because in this case the pair (m_1^+, m_2^-) has a very short inner orbit and other particles "see" the tightly bound pair (m_1^+, m_2^-) as neutral, thus forcing the system to fall apart. Our aim in this Letter is to present the rigorous and analytic proof of this screening effect, namely,

$$\frac{\mu_R}{\mu_x} \leq \frac{13 - 2\sqrt{22}}{54} \approx 0.067 \Rightarrow \text{ Instability.} \qquad (1)$$

Equation (1) manifests the screening effect for four particles. From Eq. (1) it easily follows that the hydrogen-antihydrogen molecule has no bound states and must decay into protonium and positronium. Muonic molecules $p\mu^- e^+ e^-$ and $\mu^+ \bar{p} e^+ e^-$ and $\mu^+ \mu^- e^+ e^-$ are unstable as well. And if in the hydrogen-antihydrogen system the hydrogen atom is replaced by its heavier isotopes (when deutron or tritium takes the place of the proton) the system still remains unstable. Let us compare the bound in Eq. (1) with existing numerical estimates. For the symmetric system M^+, M^-, m^+, m^- numerical calculations [3] predict instability already for $M/m > 2.2$, while Eq. (1) adopted to this particular case tells us that the system is definitely unstable for $M/m > 58.7$. Though in agreement with [3], this number is much larger than the one obtained numerically; however, the present method leaves room for improvement of the constant in Eq. (1), so that it can get closer to the number from [3]. Our derivation of Eq. (1) has its advantage of being purely analytical.

The proof of Eq. (1) is along the same line as in [10] (the basic idea goes back to Thirring [7]). The trick is after certain steps to end up in the situation where the pair of particles (m_1^+, m_2^-) stays in its ground state. This pair then generates the effective potential V_{eff} and it remains to check whether other particles have bound states in this effective potential. The ground state of the pair (m_1^+, m_2^-) is spherically symmetric and screening is incorporated into V_{eff}. The power of effective potential defines the degree of screening.

Let $q_i, \mathbf{r}_i \in \mathbb{R}^3$ denote charges and position vectors of the particles $i = 1, 2, 3, 4$. We shall work in the system of units where $\hbar = 1$. We put $q_{1,3} = +1$, and $q_{2,4} = -1$, and the interactions between the particles are $V_{ik} = q_i q_k / |\mathbf{r}_i - \mathbf{r}_k|$ (remember how the particles are ordered). The stability problem with Coulomb interactions is invariant with respect to scaling all masses [9], so we can put $\mu_x = 2$. By the end we shall rescale the masses back. Throughout the Letter we shall use the following notation: for two operators B, C the relation $B \geq C$ means that $\langle \phi | B | \phi \rangle \geq \langle \phi | C | \phi \rangle$ for any ϕ.

From now on we restrict the range of considered systems requiring $\mu_R < 3/8$ [this is weaker than in Eq. (1), so all systems described by Eq. (1) are within this range]. The strategy of our proof is the following. We start with assuming that the system is stable and derive the necessary condition for stability. After that, we shall figure out the masses for which this condition definitely does not hold, thus arriving at Eq. (1). To separate the center of mass motion we introduce the Jacobi frame [11] putting $\mathbf{x} = \mathbf{r}_2 - \mathbf{r}_1$, $\mathbf{y} = \mathbf{r}_4 - \mathbf{r}_3$, $\mathbf{R} = -a\mathbf{x} + \mathbf{r}_3 - \mathbf{r}_1 + b\mathbf{y}$, where $a = m_2^- / (m_1^+ + m_2^-)$ and $b = m_4^- / (m_3^+ + m_4^-)$ are the mass parameters invariant with respect to mass scaling. With Jacobi momenta defined as $\mathbf{p}_{x,y,R} = -i\nabla_{x,y,R}$, the Hamiltonian of the system takes the form

$$H = h_{12} + h_{34} + \frac{\mathbf{p}_R^2}{2\mu_R} + W, \qquad (2)$$

where

$$W = V_{13} + V_{14} + V_{23} + V_{24}, \qquad (3)$$

and $h_{12} = \mathbf{p}_x^2/4 - 1/x$, and $h_{34} = \mathbf{p}_y^2/(2\mu_y) - 1/y$ are the Hamiltonians of the pairs $(1, 2)$ and $(3, 4)$ (notation x is used instead of $|\mathbf{x}|$). The ground state wave function of h_{12} is $\phi_0 = \sqrt{8/\pi}\exp(-2x)$ so that $h_{12}\phi_0 = -\phi_0$. By the particle ordering, the energy threshold corresponding to dissociation into two neutral pairs is $E_{\text{th}} = -1 - \mu_y/2$, which is the sum of the binding energies of the pairs $(1, 2)$ and $(3, 4)$. Following [10] we cut off the positive part of W by introducing $W_- \equiv (|W| - W)/2$ and $W_+ \equiv (|W| + W)/2$, which results in the decomposition $W = W_+ - W_-$, where $W_\pm \geq 0$. Instead of H, we shall consider the Hamiltonian

$$\tilde{H} = h_{12} + h_{34} + \frac{\mathbf{p}_R^2}{2\mu_R} - W_-. \qquad (4)$$

(The operator $\tilde{H}$ is self-adjoint on the same domain as H; see [10].) Let us assume that H is stable; i.e., H has a bound state Ψ with the energy $E < E_{\text{th}}$. Because $\tilde{H} \leq H$ we conclude that $\langle \Psi | \tilde{H} | \Psi \rangle < E_{\text{th}} \| \Psi \|^2$. Before using this inequality let us introduce a projection operator P_0, which acts on any $f(\mathbf{x}, \mathbf{y}, \mathbf{R})$ as

$$P_0 f \equiv \phi_0(x) \int d\mathbf{x}' \phi_0(x') f(\mathbf{x}', \mathbf{y}, \mathbf{R}), \qquad (5)$$

and put $\eta = P_0 \Psi$ and $\xi = (1 - P_0)\Psi$, where obviously $\eta \perp \xi$ and $\Psi = \eta + \xi$. We shall assume that $\| \xi \| \neq 0$ (later we shall get rid of this assumption), then we are free to choose such normalization of Ψ that $\| \xi \| = 1$. Now let us rewrite the inequality $\langle \Psi | \tilde{H} | \Psi \rangle < E_{\text{th}} \| \Psi \|^2$ decomposing Ψ into $\Psi = \eta + \xi$.

$$\langle\eta|h_{34}|\eta\rangle + \langle\eta|\frac{\mathbf{p}_R^2}{2\mu_R} - W_-|\eta\rangle - \langle\eta|W_-|\xi\rangle - \langle\xi|W_-|\eta\rangle + \langle\xi|h_{12}|\xi\rangle + \langle\xi|h_{34}|\xi\rangle + \langle\xi|\frac{\mathbf{p}_R^2}{2\mu_R} - W_-|\xi\rangle < -1 - (\mu_y/2)(\|\eta\|^2 + 1), \quad (6)$$

where we have used that the terms like $\langle\eta|\mathbf{p}_y^2|\xi\rangle$ cancel because P_0 commutes with the operators $\mathbf{p}_y^2$, $\mathbf{p}_R^2$, and $1/y$. Indeed, in this case for example $\langle\eta|\mathbf{p}_y^2|\xi\rangle = \langle\eta|P_0\mathbf{p}_y^2|\xi\rangle = \langle\eta|\mathbf{p}_y^2 P_0|\xi\rangle = 0$.

We are going to rewrite Eq. (6) using lower bounds for some of its terms. From the hydrogen ground state and by the variational principle for the terms in Eq. (6) the following inequalities hold $\langle\eta|h_{34}|\eta\rangle \geq -(\mu_y/2)\|\eta\|^2$ and $\langle\xi|h_{34}|\xi\rangle \geq -\mu_y/2$. Introducing two non-negative constants, $\alpha = \sqrt{\langle\eta|W_-|\eta\rangle}$ and $\beta = \sqrt{\langle\xi|W_-|\xi\rangle}$, we get by virtue of the Schwarz inequality $|\langle\xi|W_-|\eta\rangle| \leq \alpha\beta$. It remains to figure out the bound for the term $\langle\xi|h_{12}|\xi\rangle$. From the bound spectrum of the hydrogen atom we have [7] $h_{12} \geq -P_0 - 1/4(1 - P_0)$. (Indeed, P_0 projects on the ground state of h_{12} which has the energy -1, and the energy of all other excited states is greater or equal to $-1/4$ which is the energy of the second excited state.) Hence for the first term in Eq. (6) we get the bound $\langle\xi|h_{12}|\xi\rangle \geq -1/4$. Substituting this into Eq. (6) leaves us with the main inequality

$$\langle\eta|\frac{\mathbf{p}_R^2}{2\mu_R} - W_-|\eta\rangle - 2\alpha\beta + \langle\xi|\frac{\mathbf{p}_R^2}{2\mu_R} - W_-|\xi\rangle < -\frac{3}{4}. \quad (7)$$

We shall focus on the third term on the left-hand side of Eq. (7).

First, let us prove that the inequality

$$\frac{\mathbf{p}_R^2}{2\mu_R} + QV_{14} + QV_{23} \geq -2Q^2\mu_R \quad (8)$$

holds in the operator sense for any constant $Q \geq 0$. The interactions in Eq. (8) have the form $V_{14} = -1/|\mathbf{R} - \mathbf{z}_1|$ and $V_{23} = -1/|\mathbf{R} - \mathbf{z}_2|$, where the vectors $\mathbf{z}_1 = -a\mathbf{x} - (1 - b)\mathbf{y}$ and $\mathbf{z}_2 = (1 - a)\mathbf{x} + b\mathbf{y}$ play the role of parameters. Let us denote $e(\mathbf{z}_1, \mathbf{z}_2)$ the energy of the Hamiltonian on the left-hand side of Eq. (8), where by translational invariance $e(\mathbf{z}_1 + \mathbf{a}, \mathbf{z}_2 + \mathbf{a}) = e(\mathbf{z}_1, \mathbf{z}_2)$. The function $e(\mathbf{z}_1, \mathbf{z}_2)$ can be easily recognized as the energy of the particle charge -1 and mass μ_R moving in the field of two positive charges Q located at the fixed centers $\mathbf{z}_1$ and $\mathbf{z}_2$. According to [12], $e(\mathbf{z}_1, \mathbf{z}_2)$ monotonically increases with $|\mathbf{z}_1 - \mathbf{z}_2|$, hence the minimum energy is attained when both centers of attraction coincide, i.e., when $\mathbf{z}_1 = \mathbf{z}_2 = 0$. This makes the sum of interaction terms in Eq. (8) equal to $-2Q/R$. The right-hand side of Eq. (8) is the energy of the particle mass μ_R in this potential. From Eq. (8) using the obvious inequality $-W_- \geq V_{14} + V_{23}$ we find that for any $Q \geq 0$ and $\chi(\mathbf{x}, \mathbf{y}, \mathbf{R})$,

$$\langle\chi|\frac{\mathbf{p}_R^2}{2\mu_R} - QW_-|\chi\rangle \geq -2Q^2\mu_R\|\chi\|^2. \quad (9)$$

With the help of Eq. (9) we get the following chain of inequalities

$$\begin{aligned}\langle\xi|\frac{\mathbf{p}_R^2}{2\mu_R} - W_-|\xi\rangle &= \max_{\lambda\geq -1}\left[\langle\xi|\frac{\mathbf{p}_R^2}{2\mu_R} - (\lambda+1)W_-|\xi\rangle + \lambda\beta^2\right] \\ &\geq \max_{\lambda\geq -1}[-2(\lambda+1)^2\mu_R + \lambda\beta^2] \\ &= \frac{\beta^4}{8\mu_R} - \beta^2, \end{aligned} \quad (10)$$

where we have added and subtracted the term $\lambda\beta^2 = \lambda\langle\xi|W_-|\xi\rangle$. Substituting Eq. (10) into Eq. (7) leaves us with the inequality

$$\langle\eta|\frac{\mathbf{p}_R^2}{2\mu_R} - W_-|\eta\rangle + \frac{\beta^4}{8\mu_R} - \beta^2 - 2\alpha\beta < -\frac{3}{4}. \quad (11)$$

The following inequality always holds

$$\frac{\beta^4}{8\mu_R} - \beta^2 - 2\alpha\beta + \frac{3}{4} \geq -\left(\sqrt{\frac{3}{8\mu_R}} - 1\right)^{-1}\alpha^2. \quad (12)$$

To see that Eq. (12) is true it suffices to take all terms to the left-hand side and minimize over α (the minimum is attained at the point of zero derivative with respect to α). Substituting Eq. (12) into Eq. (11) and using $\alpha^2 = \langle\eta|W_-|\eta\rangle$ makes us conclude that the system of four unit charges for $\mu_R < 3/8$ is stable only if

$$\langle\eta|\frac{\mathbf{p}_R^2}{2\mu_R} - \{1 + [\sqrt{3/(8\mu_R)} - 1]^{-1}\}W_-|\eta\rangle < 0. \quad (13)$$

It remains to consider the case when $\|\xi\| = 0$. It is easy to see that in this case the substitution $\Psi = \eta$ into the inequality $\langle\Psi|\tilde{H}|\Psi\rangle < E_{\text{th}}\|\Psi\|^2$ leads to the condition even more stringent than Eq. (13).

It makes sense to introduce the effective potential $V_{\text{eff}}(\mathbf{y}, \mathbf{R}) = \int d\mathbf{x}|\phi_0|^2 W_-$. The function η has the factorized form $\eta = \phi_0(\mathbf{x})f(\mathbf{y}, \mathbf{R})$. Substituting this into Eq. (13) and performing the internal integration over $\mathbf{R}$ and $\mathbf{x}$ tells us that Eq. (13) would be broken if for all fixed $\mathbf{y}$,

$$\frac{\mathbf{p}_R^2}{2\mu_R} - \{1 + [\sqrt{3/(8\mu_R)} - 1]^{-1}\}V_{\text{eff}} \geq 0, \quad (14)$$

where the operator inequality Eq. (14) is understood on the functions depending on $\mathbf{R}$ alone. Summarized, if $\mu_R < 3/8$ and Eq. (14) holds for all fixed $\mathbf{y}$, the system is unstable.

We shall make one simplification, which helps carrying out all calculations analytically. We have $W = W_1 + W_2$, where $W_1 = V_{14} + V_{24}$ and $W_2 = V_{13} + V_{23}$. Obviously $W_- \leq (W_1)_- + (W_2)_-$ and hence $V_{\rm eff} \leq V_{\rm eff}^{(1)} + V_{\rm eff}^{(2)}$, where $V_{\rm eff}^{(i)} = \int d\mathbf{x}|\phi_0|^2(W_i)_-$. Breaking the kinetic energy term in Eq. (14) into two equal parts and substituting $V_{\rm eff} \leq V_{\rm eff}^{(1)} + V_{\rm eff}^{(2)}$ we deduce that the system is unstable if both of the following inequalities are satisfied independently for all fixed $\mathbf{y}$

$$\mathbf{p}_R^2 - 4\mu_R\{1 + [\sqrt{3/(8\mu_R)} - 1]^{-1}\}V_{\rm eff}^{(i)} \geq 0 \tag{15}$$

for $i = 1, 2$. Now we can apply the explicit calculation from [10], where we have shown that the following inequality

$$\int |\phi_0|^2[-|a\mathbf{x} - \mathbf{y}|^{-1} + |(1-a)\mathbf{x} + \mathbf{y}|^{-1}]_- d\mathbf{x} < \frac{3}{16y^2} \tag{16}$$

holds for all $a \in [0, 1]$ [this is Eq. (16) in Ref. [10]]. Through Eq. (16) we derive the upper bounds $V_{\rm eff}^{(i)} \leq (3/16)|\mathbf{R} + c_i\mathbf{y}|^{-2}$, where $c_1 = (1-b)$ and $c_2 = -b$. Now we simply replace $V_{\rm eff}^{(i)}$ in Eq. (15) with these upper bounds, which makes both inequalities stronger. It is known [13,14] that $\mathbf{p}_R^2 - \lambda|\mathbf{R} + c_i\mathbf{y}|^{-2} \geq 0$ for $\lambda \leq 1/4$ (by translational invariance, the value of $\mathbf{y}$ does not play a role and one can put $\mathbf{y} = 0$). Thus both inequalities Eq. (15) are satisfied if $3\mu_R\{1 + [\sqrt{3/(8\mu_R)} - 1]^{-1}\} \leq 1$. Solving this simple inequality and rescaling the masses tells us that the system is unstable if $\mu_R \leq (13 - 2\sqrt{22})\mu_x/54$, which proves Eq. (1). Notice that the final bound on the effective potential is proportional to R^{-2}, which is similar to the dipole interaction and makes an interesting parallel to [13]. The constant in Eq. (1) can be improved if everything is extracted from Eq. (14); i.e., one has to calculate precisely $V_{\rm eff}$. We preferred to simplify by splitting W into two terms because this makes the whole derivation analytical. Let us also remark that instability in Eq. (1) means that there is no bound state either below or *at* the threshold. Indeed, if we would have $H\Psi = E_{\rm th}\Psi$ then, because one can choose $\Psi > 0$ in the ground state, we immediately get $\langle\Psi|\tilde{H}|\Psi\rangle < E_{\rm th}||\Psi||^2$ which was the starting point of our analysis.

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