Stability of Three Unit Charges. Necessary Conditions.

D.K. Gridnev, C. Greiner, and W. Greiner

Institut für Theoretische Physik, Robert-Mayer-Str. 8-10, D-60325 Frankfurt am Main, Germany

We consider the stability of three Coulomb charges \{+1, -1, -1\} with finite masses in the framework of nonrelativistic quantum mechanics. A simple physical condition on masses is derived to guarantee the absence of bound states below the dissociation thresholds. In particular this proves that certain negative muonic ions are unstable, thus extending the old result of Thirring to the actual values of all masses. The proof is done by reducing the initial problem to the question of binding of one particle in some effective potential.

I. INTRODUCTION

The stability of three particles with pure Coulomb forces is an old and extensively studied problem, this is to explain why certain ions and molecules stay as a whole and some dissociate into a bound pair and a single particle. Under stability of the Hamiltonian \(H\) we shall understand the existence of a bound state with the energy strictly less than \(\inf \sigma_{\text{ess}}(H)\), i.e. a stationary state below all dissociation thresholds. As a quantum system three particles with Coulomb interactions demonstrate interesting behavior. It is known that three charges \(\{1 + \varepsilon, -1, -1\}\) for any \(\varepsilon > 0\) form the system, which is stable regardless of mass values. However at \(\varepsilon = 0\) the situation abruptly changes and due to the screening effect not all systems remain stable. The typical example is the unstable muonic hydrogen ion \(p\mu^- e^-\), where the heavy muon is tightly bound to the proton and screens the positive charge for the electron. This interesting effect is well studied, in particular it has been proved\(^2\) that for equal dissociation thresholds the system remains stable (Refs.\(^3,4\) explain very well how stability depends on masses and charges).

Among the instability proofs for three unit charges the most appealing is that of Thirring, which does not require any numerical calculations. Thirring considered a negative hydrogen ion with an infinitely heavy proton, and proved that such negative ion is unstable when its second negatively charged particle is lighter than electron by a factor larger than \(\pi\) (\(\pi\) can be replaced with a better constant 1.57). In his method Thirring exploited the fact that the ground state in the hydrogen atom is substantially separated from other states in its spectrum (the non-degenerate

*Electronic address: dimagridnev@yahoo.com
energy levels have $1/n^2$ dependence), and thus its role becomes emphasized. This suggests an idea to move the problem to the space spanned by the projector $P_0 = |\phi_0\rangle\langle\phi_0| \otimes 1$, where $\phi_0$ is the ground state of Hydrogen. After estimating the part of the repulsion, which is present in this space, the problem reduces to checking the binding of one particle in some effective potential. The contribution from the attractive interaction term coming from additional particle is easy to treat because it commutes with $P_0$. Yet this is no longer true if one considers particles of finite mass or any system of four particles.

Thirring’s bound was improved and it was shown that the muonic ion $p\mu^-e^-$ is unstable for actual values of all masses. However this extension (Eq. 24 in Ref. 3) is weak in the sense that it fails when the second particle is heavy compared to other particles. (For a physical example, it does not prove that the ion $\mu^- pe^+$ is unstable, yet we shall prove it here). This extension still uses Thirring’s treatment of repulsion and it is unclear how one could extend it to four particles. Armour with his method proved the instability of such systems as positron-hydrogen-atom $e^- pe^+$ and $\mu^- pe^+$, but this method requires certain numerical assistance. It also bases on the separation of variables in the problem of two fixed centers, which makes it inapplicable to four particles because the variables do not separate even in the case of three fixed centers.

Here we follow the Thirring’s idea but the nucleus does not have to be infinitely heavy. The derived physical condition restricts the ratio of Jacobi masses, which makes the system stable. It can be used in conjunction with Thirring’s result and convexity properties of stability curve for a reasonable determination of stability area free from any numerics. The present method has an important advantage in that it admits generalization to four particles. It should be mentioned that both Thirring’s method and the new one share the same deficiency, namely, they are not applicable when the dissociation thresholds in the system are close or equal (e.g. when two like charges have equal masses). In particular, using such methods one cannot prove the “overheating” effect, when a system with charges $\{+1, -q, -q\}$ and equal masses loses its binding for some $q > 1$. Nowadays various charged particles are produced in laboratories and it is, of course, of interest to know the principles behind formation of exotic atoms or molecules. All this motivates the present analysis.

II. FROM THREE PARTICLES TO ONE IN EFFECTIVE POTENTIAL

Let $m_i, q_i, r_i \in \mathbb{R}^3$ denote masses, charges and position vectors of particles $i = 1, 2, 3$. We put $q_1 = +1$, and $q_{2,3} = -1$, and the interactions between the particles are $V_{ik} = q_i q_k / |r_i - r_k|$. We enumerate the particles in such a way, that the particles $(1,2)$ form the lowest dissociation
threshold. The stability problem with Coulomb interactions is invariant with respect to scaling all masses, so we can put \( \hbar = 1 \). We separate the center of mass motion in the Jacobi frame by putting \( \mathbf{x} = \mathbf{r}_1 - \mathbf{r}_2 \) and \( \mathbf{y} = \mathbf{r}_3 - \mathbf{r}_1 + a\mathbf{x} \), where \( a = m_2/(m_1 + m_2) \) is the mass parameter invariant with respect to mass scaling. The reduced masses and Jacobi momenta are respectively \( \mu_x = m_1m_2/(m_1 + m_2) \), \( \mu_y = m_3(m_1 + m_2)/(m_1 + m_2 + m_3) \) and \( p_{x,y} = -i\nabla_{x,y} \). It is convenient to scale all masses so that \( \mu_x = 2 \). (In Sec. [V] we shall rescale them back). The Hamiltonian for the system on the tensor product space \( L_2(\mathbb{R}^3) \otimes L_2(\mathbb{R}^3) \) is

\[
H = h_{12} \otimes 1 + 1 \otimes \frac{p_y^2}{2\mu_y} + W
\]

where

\[
W = V_{13} + V_{23} = -\frac{1}{\lvert a\mathbf{x} - \mathbf{y} \rvert} + \frac{1}{\lvert (1-a)\mathbf{x} + \mathbf{y} \rvert}
\]

and \( h_{12} = p_x^2/4 - 1/x \) is the Hamiltonian of the pair of particles (1,2) (notation \( x \) is used instead of \( \lvert \mathbf{x} \rvert \)). The ground state wave function of \( h_{12} \) is \( \phi_0 = \sqrt{8/\pi} \exp(-2x) \) so that \( h_{12}\phi_0 = -\phi_0 \).

The Hamiltonian \( H \) is self-adjoint on \( D(H) = H^2(\mathbb{R}^6) \) (square integrable functions having partial derivatives up to the second order in the weak distributional sense) and by the HVZ theorem \( \sigma_{ess}(H) = [-1, \infty) \). We split positive and negative parts of \( W \) by introducing \( W_- := (\lvert W \rvert - W)/2 \) and \( W_+ := (\lvert W \rvert + W)/2 \) and we have \( W = W_+ - W_- \), where \( W_\pm \geq 0 \). Instead of \( H \) we shall consider the Hamiltonian

\[
\tilde{H} = h_{12} \otimes 1 + 1 \otimes \frac{p_y^2}{2\mu_y} - W_-
\]

Note that the part \( W_- \) can also be expressed as

\[
W_- = -(V_{13} + V_{23}F(\mathbf{x}, \mathbf{y}))
\]

where \( F = 1 \) when \( \lvert V_{13} \rvert \geq \lvert V_{23} \rvert \) and \( F = \lvert V_{13} \rvert / \lvert V_{23} \rvert \) when \( \lvert V_{13} \rvert \leq \lvert V_{23} \rvert \), and we have \( 0 \leq F \leq 1 \). Because \( \lVert V_{23}F\phi \rVert \leq \lVert V_{23}\phi \rVert \) we can directly apply Kato’s theorem on self-adjointness of atomic Hamiltonians and find out that \( \tilde{H} \) is self-adjoint on \( D(\tilde{H}) = D(H) \). We cannot though directly apply the HVZ theorem to locate \( \inf \sigma_{ess}(\tilde{H}) \) but we observe that the following inequality holds

\[
(H - V_{23}) \leq \tilde{H} \leq H.
\]

Here \( (H - V_{23}) \) is the original Hamiltonian without repulsion, which is bounded from below and by the HVZ theorem \( \inf \sigma_{ess}(H - V_{23}) = -1 \). Thus from the min-max principle we get \( \inf \sigma_{ess}(\tilde{H}) = -1 \).

Now let us assume that \( H \) is stable, i.e. \( H \) has a bound state with the energy less than \(-1 \). Because \( \tilde{H} \leq H \) from the variational principle we conclude that \( \tilde{H} \) also has a bound state \( \Psi \in D(H) \).
with the energy below \( \inf \sigma_{ess}(\tilde{H}) = -1 \) which means
\[
\tilde{H} \Psi = (-1 - \delta) \Psi
\] (4)
where \( \delta > 0 \) is the extra binding energy. Let us introduce a projection operator \( P_0 = |\phi_0\rangle \langle \phi_0| \otimes 1 \) \((P_0 : \mathcal{D}(H) \to \mathcal{D}(H))\) and put \( \eta := P_0 \Psi \) and \( \xi := (1 - P_0) \Psi \), where obviously \( \eta \perp \xi \) and \( \Psi = \eta + \xi \) and \( \eta, \xi \in \mathcal{D}(H) \). Taking the scalar product of each side of (4) with \( \eta \) and \( \xi \) we obtain
\[
\langle \eta | 1 \otimes \frac{P_y^2}{2\mu_y} - W_- | \eta \rangle - \langle \eta | W_- | \xi \rangle = -\delta \| \eta \|^2
\] (5)
\[
\langle \xi | h_{12} \otimes 1 | \xi \rangle + \langle \xi | 1 \otimes \frac{P_y^2}{2\mu_y} - W_- | \xi \rangle - \langle \xi | W_- | \eta \rangle = (-1 - \delta) \| \xi \|^2
\] (6)
where we have used \( \langle \eta | 1 \otimes \frac{P_y^2}{2\mu_y} | \xi \rangle = 0 \) because \( P_0 \) and \( 1 \otimes \frac{P_y^2}{2\mu_y} \) commute. We shall assume that \( \| \eta \|, \| \xi \| \neq 0 \) (we shall get rid of this assumption in Theorem 1), then we are free to choose such normalization of \( \Psi \) that \( \| \xi \| = 1 \).

From the bound spectrum of \( h_{12} \) we have \( h_{12} \otimes 1 \geq -P_0 - 1/4(1 - P_0) \), hence for the first term in (6) we get the bound \( \langle \xi | h_{12} \otimes 1 | \xi \rangle \geq -1/4 \). 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 \( |\langle \xi | W_- | \eta \rangle| \leq \alpha \beta \).

Now we can rewrite Eq. (5)–(6) to obtain the main pair of inequalities
\[
\langle \eta | 1 \otimes \frac{P_y^2}{2\mu_y} - W_- | \eta \rangle - \alpha \beta < 0
\] (7)
\[
\langle \xi | 1 \otimes \frac{P_y^2}{2\mu_y} - W_- | \xi \rangle - \alpha \beta < -\frac{3}{4}
\] (8)
Using the second inequality we shall find \( \max \beta/\alpha \) and by substituting this value into (7) we shall formulate the stability condition.

**Lemma 1.** Suppose that Eq. (5) holds and \( \mu_y < 3/2 \), then the following inequality is true
\[
\beta < \left( \frac{3}{2\mu_y} - 1 \right)^{-1} \alpha
\] (9)

**Proof.** First, let us show that for \( A \geq 0 \)
\[
\inf_{\chi \in \mathcal{D}(H)} \langle \chi | 1 \otimes \frac{P_y^2}{2\mu_y} - AW_- | \chi \rangle \geq -\frac{A^2 \mu_y}{2}
\] (10)
It suffices to prove this for \( \chi \in C_0^\infty(\mathbb{R}^6) \). Using (3) from the variational principle we get
\[
\langle \chi | 1 \otimes \frac{P_y^2}{2\mu_y} - AW_- | \chi \rangle \geq \int dx \int dy \chi^\ast(x, y) \left( \frac{P_y^2}{2\mu_y} - \frac{A}{|ax - y|} \right) \chi(x, y)
\]
\[
\geq -\frac{A^2 \mu_y}{2} \int dx \int dy |\chi|^2(x, ax + y) = -\frac{A^2 \mu_y}{2} \| \chi \|^2
\] (11)
from which (10) follows and where we have used the explicit expression for the ground state energy of the hydrogen atom. (Using an appropriate set of trial functions it is easy to show that there is an equality sign in (10), but we do not need this for our purposes). Now using (10) we obtain the following chain of inequalities

$$\inf_{\xi \in \mathcal{D}(H)} \frac{\langle \xi | 1 \otimes \frac{p^2_y}{2\mu_y} - W_- | \xi \rangle}{\|\xi\| = 1} = \max_{\lambda \geq -1} \inf_{\xi \in \mathcal{D}(H), \|\xi\| = 1} \left( \langle \xi | 1 \otimes \frac{p^2_y}{2\mu_y} - (\lambda + 1)W_- | \xi \rangle + \lambda \beta^2 \right)$$

$$\geq \max_{\lambda \geq -1} \inf_{\xi \in \mathcal{D}(H), \|\xi\| = 1} \left( \langle \xi | 1 \otimes \frac{p^2_y}{2\mu_y} - (\lambda + 1)W_- | \xi \rangle + \lambda \beta^2 \right) \geq \max_{\lambda \geq -1} (\lambda \beta^2 - (\lambda + 1)^2 \mu_y/2)$$

$$= \frac{\beta^4}{2\mu_y} - \beta^2$$

Substituting this result into (8) and putting $\alpha = s\beta$ we obtain

$$\frac{\beta^4}{2\mu_y} - (s + 1)\beta^2 < -\frac{3}{4}$$

Now simply minimizing the left-hand side of (12) over $\beta^2$ we obtain the lower bound on $s$, which gives us Eq. (9).

It is worth noting that the relation in Lemma is a version of the uncertainty principle, when $\beta^2$ grows, the kinetic energy term grows faster like $\beta^4$. Let us introduce an effective potential $V_{eff}(y) := \int d\mathbf{x} |\phi_0|^2 W_-$. We formulate the result as

**Theorem 1.** If the system of three charges is stable and $\mu_y < 3/2$ then the particle with mass $\mu_y$ must have a bound state in the potential $- (1 + (\sqrt{3/2\mu_y} - 1)^{-1}) V_{eff}$.

**Proof.** We have $\|\eta\|, \|\xi\| \neq 0$. The function $\eta$ has the factorized form $\eta = \phi_0(x)f(y)$, where $f \in H^2(\mathbb{R}^3), \|f\| \neq 0$. By substituting (9) into (7) and using expressions for $\alpha^2$ and $\eta$ we get the necessary condition for stability

$$\langle f | \frac{p^2_y}{2\mu_y} - \left(1 + (\sqrt{3/2\mu_y} - 1)^{-1}\right) V_{eff} | f \rangle < 0$$

(13)

In the next section we shall study $V_{eff}(y)$ and show that it is a continuous function decaying like $1/y^2$. Inequality (13) means that a particle having mass $\mu_y$ has a bound state in this potential.

Now let us complete the proof considering the case when either $\xi = 0$ or $\eta = 0$. If $\xi = 0$ we have $\beta = 0$ and substituting this into (7) we get a condition more stringent than Eq. (13). If $\eta = 0$ we have $\|\xi\| = 1$ and $\alpha = 0$, substituting this into (8) and using (10) for $\mu_y < 3/2$ results in the contradiction.
III. BINDING IN EFFECTIVE POTENTIAL

In this section we shall analyze the effective potential and find out at which values of the coupling constant $\lambda$ the Hamiltonian $p^2_y - \lambda V_{\text{eff}}$ may have bound states. It turns out that the effective potential in our case has a nonphysical term, which is a long-range attraction of the type $1/y^2$. This nonphysical behavior stems from cutting off the positive part of the potential and results in the infinite number of bound states at the point of binding (that is why it is meant nonphysical). But as it is well-known since the result of Hilbert and Courant, even this long-range attraction does not guarantee binding, for $\lambda \max_y y^2 V_{\text{eff}}(y) \leq 1/4$ the inequality $p^2_y - \lambda V_{\text{eff}} \geq 0$ holds, i.e. no binding occurs, (see also the proof in Ref. 8, vol. 2). Thus the non-trivial critical coupling constant exists, and we have to determine it. On the other hand, in such potentials short-range repulsive terms do not play any role for binding. It would be of interest to get rid of this nonphysical behavior in the future (pay attention that the Thirring’s effective potential behaves at infinity like $1/y^3$).

To calculate $V_{\text{eff}}$ we must cut off the positive part of $W$. From (11) $W \leq 0$ is equivalent to $\cos \theta \geq x/(\omega y)$, where $\omega = (a - 1/2)^{-1}$ and $\cos \theta = x \cdot y / xy$. We shall consider separately two cases $a > 1/2$ and $a \leq 1/2$.

A. Case when $a > 1/2$

The integration is simpler in this case. After direct integration in spherical coordinates over the area where $\cos \theta \geq x/(\omega y)$ we obtain

$$V_{\text{eff}}(y) = 16y^2 \int_0^\omega ds \ se^{-4sy} \left( \frac{\sqrt{a(1-a)s^2 + 1}}{a(1-a)} - \frac{|as - 1|}{a} - \frac{(1-a)s + 1}{1-a} \right)$$

$$= \frac{16y^2}{a(1-a)} \int_0^\omega ds \ se^{-4sy} (\sqrt{a(1-a)s^2 + 1} - 1) + U$$

where

$$U = 32y^2 \int_{1/a}^\omega ds \ se^{-4sy} (1/a - s) < 0$$

Now we do not have to carry out integration in $[15]$, it is enough to see that it is a short-range repulsion, which does not play a role in our case. To calculate the first term in $[14]$ we use $\sqrt{a(1-a)s^2 + 1} \leq 1 + a(1-a)s^2/2$ to get

$$V_{\text{eff}} < 8y^2 \int_0^\omega ds \ s^3 e^{-4sy} < \frac{3}{16y^2}$$

(16)
where after the integration we have dropped the short-range negative terms. Finally, we have
\[ p_y^2 - \lambda V_{eff} \geq p_y^2 - \lambda(3/16)y^{-2}. \]
The following inequality holds \( p_y^2 - (1/4)y^{-2} \geq 0. \) Thus in the case of binding, i.e. when such \( f \) exists that \( \langle f | p_y^2 - \lambda V_{eff} | f \rangle < 0, \) we must have \( \lambda > 4/3. \) Comparing this with (13) we obtain that three charges form unstable system if \( \mu_y < 3/2 \) and
\[
2\mu_y \left( 1 + \left( \sqrt{3/2\mu_y} - 1 \right)^{-1} \right) < 4/3 \tag{17}
\]
Solving this simple inequality tells us that the system is unstable when \( \mu_y < 2(11 - 2\sqrt{10})/27 \simeq 0.3463. \)

**B. Case when \( a \leq 1/2 \)**

First let us take \( a < 1/2. \) We shall write \( W(a) \) instead of \( W \) to point out the dependence on parameter \( a. \) We can alleviate the integration noting that \( W(a) = -W(1-a), \) thus we have
\[ W_(a) = (W(1-a))_+ = W_+(1-a) = W(1-a) + W_-(1-a). \]
From this we conclude \( V_{eff}(a) = -W(a) + V_{eff}(1-a). \) The additional integral \( W(a) := \int dx |\phi|^2W \) is easy to calculate and \( V_{eff}(1-a) \) for \( a < 1/2 \) we have already calculated. We obtain
\[
-W(a) = 16y^2 \int_0^\infty ds e^{-4sy}s \left( \left( \frac{1}{a} - \frac{1}{1-a} \right) + \left| s - \frac{1}{1-a} \right| - \left| s - \frac{1}{a} \right| \right)
\]
\[
= 32y^2 \int_{1/(1-a)}^{1/a} ds e^{-4sy} \left( s^2 - \frac{s}{1-a} \right) + 32y^2 \int_{1/a}^\infty ds e^{-4sy} \left( \frac{1}{a} - \frac{1}{1-a} \right) \tag{18}
\]
Using (14), (15) and approximation for the square root \( \sqrt{a(1-a)s^2 + 1} \leq 1 + a(1-a)s^2/2 \) gives us
\[
V_{eff}(1-a) \leq 8y^2 \int_0^{\omega} ds s^3 e^{-4sy} + 32y^2 \int_{1/(1-a)}^{\omega} ds e^{-4sy} \left( s - \frac{s}{1-a} \right) \tag{19}
\]
Summing (18) and (19) and calculating the integrals explicitly gives us the following expression for \( a < 1/2 \)
\[
V_{eff} < \frac{3}{16y^2} - e^{-4y/a} \left[ \frac{8(1-a)y}{a^2} + 2 \frac{2-a}{a} + \frac{1}{y} \right]
\]
\[
- e^{4\omega} \left[ -2\omega(\omega + 2)^2 + (3\omega/2 + 1)(\omega + 2) - \frac{1}{y}(3\omega/4 + 1) + \frac{3}{16y^2} \right] \tag{20}
\]
For \( a < 1/2 \) we have \( \omega < -2, \) and it is easily seen that all terms in square brackets are positive (this leads again to short-range potentials), meaning that \( V_{eff} < (3/16)y^{-2}, \) which gives the same condition for stability as (17). We do not consider explicitly \( a = 1/2, \) it is done analogously and also results in (17).
IV. SUMMARY

We have initially scaled all masses $m_i \rightarrow 2m_i/\mu_x$, making $\mu_x = 2$. Now rescaling it back we get through (17) that the system of three charges is unstable if $\mu_y/\mu_x < (11 - 2\sqrt{10})/27 \simeq 0.1732$. In the case of infinitely heavy nucleus this is $m_3/m_2 < 0.1732$, which is worse than the refined\textsuperscript{3,6} Thirring’s estimate $m_3/m_2 < 1/1.57$. The accuracy is lost at the point of cutting the positive part of the potential, which induces a long-range attraction. However this is more than enough to prove that the muonic ions $p\mu^-e^-$ or $\mu^-pe^+$ are unstable for the actual values of all three masses.

The case of four unit charges $\{+1, +1, -1, -1\}$ is treated similarly but the calculations are more involved\textsuperscript{11} and results would be published elsewhere. Let us also stress that the obtained condition is physical. Both Jacobi masses determine Bohr radii for the particle orbits, the orbit within the pair of particles $(1,2)$ and the orbit for the third particle in the field of this pair with respect to the pair’s center of mass. If the orbit of one negative particle is outdistanced then the attraction from the positive charge is screened off by the other negative particle and the system becomes unbound.

\textsuperscript{1} W. Thirring, \textit{Lehrbuch der Mathematischen Physik}, Springer–Verlag/Wien 1994, vol. 3
\textsuperscript{2} R.N. Hill, J. Math. Phys., 18, 2316 (1977)
\textsuperscript{3} A. Martin, J.M. Richard and T.T. Wu, Phys. Rev. A46, 3697 (1992)
\textsuperscript{4} A. Martin, J.M. Richard and T.T. Wu, Phys. Rev. A52, 2557 (1995)
\textsuperscript{5} E. A. G. Armour, J. Phys. B11, 2803 (1978); J. Phys. B16, 1295 (1983)
\textsuperscript{6} V. Glaser, H. Grosse, A. Martin and W. Thirring, in \textit{Studies in Mathematical Physics – Essays in Honor of Valentine Bargmann}, Princeton University Press, Princeton, NJ, 169 (1976)
\textsuperscript{7} A. Messiah, \textit{Quantum Mechanics}, North Holland Publishing, (1964)
\textsuperscript{8} M. Reed and B. Simon, \textit{Methods of Modern Mathematical Physics}, vol. 2-4, Academic Press (1978)
\textsuperscript{9} R. Courant and D. Hilbert, \textit{Methods of Mathematical Physics}, Interscience Publishers, New York, (1953), vol. 1, p. 446
\textsuperscript{10} H. van Haeringen, J. Math. Phys. 19, 2171 (1978)
\textsuperscript{11} D.K. Gridnev and C. Greiner, to appear in Phys. Rev. A