Stability of three-and four-charge systems

Jean-Marc Richard†

Institut de Physique Nucléaire
Université Claude Bernard–CNRS-IN2P3
4, rue Enrico Fermi, F–69622 Villeurbanne cedex, France

and

Institut des Sciences Nucléaires‡
Université Joseph Fourier–CNRS-IN2P3
53, avenue des Martyrs, F–38026 Grenoble cedex, France

Abstract

A brief review is presented of the stability domain of three- and four-charge ground-states when the constituent masses vary. Rigorous results are presented, based on the scaling behavior and the convexity properties deduced from the variational principle. They are supplemented by accurate numerical computations.

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†E-mail: Jean-Marc.Richard@isn.in2p3.fr
‡Permanent address
1 Three unit-charge systems

Beyond hydrogenic atoms, the simplest systems in molecular physics consist of three unit charges, \( \pm(1, -1, -1) \). The Hamiltonian reads

\[
H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{p_3^2}{2m_3} - \frac{e^2}{r_{12}} - \frac{e^2}{r_{13}} + \frac{e^2}{r_{23}}. \tag{1}
\]

A non-relativistic point-charge interaction is assumed, and everything else is neglected: relativistic corrections, finite-size effects, annihilation, strong interaction, etc.

Nevertheless, as pointed out by Thirring [1], it is not completely obvious why some systems are stable, e.g., \( \text{H}^+_2 = (p, p, e^-) \), \( \text{Ps}^- = (e^+, e^-, e^-) \) or \( \text{H}^- = (p, e^-, e^-) \), while others, such as \( (p, \bar{p}, e^-) \) or \( (e^-, p, e^+) \), immediately dissociate into a neutral atom and an isolated charge.

One can use the scaling properties of (1) and similar Hamiltonians to choose \( \bar{\hbar} = e^2 = 1 \), as well as \( \sum \alpha_i = 1 \), where \( \alpha_i = 1/m_i \) is the inverse mass of particle \( i \). It is natural to use inverse masses, as the Hamiltonian depends linearly upon them. The condition \( \sum \alpha_i = 1 \) is reminiscent of energy conservation in three-body decays, any possible configuration of which can be represented in a “Dalitz plot”, which is an equilateral triangle of unit height. Each inverse mass is read as the distance to a side, as shown in Fig. 1.

![Figure 1: The domain of normalized inverse masses \( \alpha_i \).](image1)

![Figure 2: Schematic shape of the stability domain.](image2)

Initially, some incorrect results were obtained for these systems, though these were sometimes based on very astute reasoning. It is, indeed, a more
delicate operation to estimate numerically where the stability frontier is than
to calculate the binding energy of a system whose stability is well established.
Recent numerical calculations are, however, very accurate and reliable. See,
e.g., Refs. [2, 3, 4] for some examples and the results in the literature, and
Ref. [5] for a comprehensive survey. If one summarizes the results of the
literature, one finds that the stable configurations belong to a band around
the symmetry axis $m_2 = m_3$ where like-sign charges bear the same mass.

The shape of the stability domain, as schematically pictured in Fig. 2,
results from three basic properties [6]:

1. Any state along the symmetry axis is stable. This was shown by Hill
   using the trial wave function
   \[ \Psi = \exp \left( -ar_{12} - br_{13} \right) + \{a \leftrightarrow b\}, \tag{2} \]
   where the possibility of having $a \neq b$ is crucial, as already noted
   by Chandrasekhar [8] for H$^-$ and Hylleraas [9] for Ps$^-$. Note that
   if a wave function with only an adjustable effective charge $Z_e$, i.e.,
   $\Psi \propto \exp(-Z_e(r_{12} + r_{13}))$, or even more generally, any factorized wave
   function $f(r_{12})f(r_{13})$ is used, it is not possible to demonstrate the sta-
   bility of H$^-$ [10]; one needs the anticorrelation $a \neq b$, or an explicit $r_{23}$
   dependence, or both.

2. Each instability region is convex. This results from the convexity prop-
   erties of the ground-state energy, after suitable rescaling such that the
   threshold energy $E(m_1^+, m_2^-)$ (or $E(m_1^-, m_3^-)$ on the other side) is kept
   constant.

3. Each instability region has as a star shape with respect to $A_2$ or $A_3$.
   For instance, if one draws a line from $A_3$ toward the symmetry axis, it
   corresponds, after rescaling, to increasing $m_3$ while the threshold energy
   $E(m_1^+, m_2^-)$ remains constant. Increasing $m_3$ decreases the three-body
   binding energy and thus improves stability.

An application of this approach can be made when searching the critical
masses for which stability disappears, for instance,
\[ \alpha : (m_\alpha^+, \infty^-, 1^-) \quad \beta : (\infty^+, m_\beta^-, 1^-) \quad \gamma : (1^+, m_\gamma^-, 1^-). \tag{3} \]

In Fig. 3, one can see that a safe (lower) bound on $m_\alpha$ and a safe (upper)
bound on $m_\beta$ result in a straight line entirely in an instability domain. It
Figure 3: Some critical points of interest.

Figure 4: Schematic shape of the stability domain of \((m_1^+, m_2^+, m_3^-, m_4^-)\) states in the tetrahedron of normalized inverse masses \(\alpha_i = m_i^{-1}\), with \(\sum \alpha_i = 1\).

intersects at \(\gamma'\) the \(m_1 = m_3\) axis, this providing a upper bound for the critical mass \(m_\gamma\), which turns out to be better than the limits obtained by direct studies of the particular configurations \((1^+, m^-, 1^-)\). In other words, global considerations on the triangle of stability are sometimes more powerful than local studies.

2 Four unit-charge systems

Consider now \((m_1^+, m_2^+, m_3^-, m_4^-)\) systems, whose Hamiltonian reads

\[
H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{p_3^2}{2m_3} + \frac{p_4^2}{2m_4} - \frac{e^2}{r_{13}} - \frac{e^2}{r_{23}} - \frac{e^2}{r_{14}} - \frac{e^2}{r_{24}} + \frac{e^2}{r_{12}} + \frac{e^2}{r_{34}},
\]

with, again, some scaling properties, so that \(\sum \alpha_i = 1\) can be imposed: each configuration is a point in a regular tetrahedron, and the inverse constituent masses \(\alpha_i = m_i^{-1}\) represent the distances to the faces.
The lowest threshold consists of either two atoms or one three-body ion and an isolated charge. The lowest two-atom state is obtained by combining the heaviest of the positive charges $m_1$ and $m_2$ with the heaviest of the negative charges $m_3$ and $m_4$, and allowing the two lightest masses to form a second atom. This can be seen explicitly from the Bohr formula, but this is a more general results for any given potential, as shown in Refs. [11, 12]. If for instance the first three particles are heavy and form a stable ion, then the lowest threshold is $(m_1^+, m_2^-, m_3^-) + m_4^-$. As the ion attracts the last charge with a potential that is asymptotically attractive and Coulombic, and thus supports many bound states, one is sure in such situation that the four-body system is stable. In practice, stability is guaranteed by finding a wave function whose expectation value for $H$ is smaller than the energy of the lowest two-atom threshold.

For the equal-mass case, i.e., the positronium molecule $\text{Ps}_2$, this was done in 1947 by Hylleraas and Ore [13]. Later on, it was realized that the stability of $\text{Ps}_2$ implies that of all hydrogen-like configurations $(M^+, M^+, m^-, m^-)$, $\forall M/m$. This includes the ordinary hydrogen molecule, starting from $M = m$, instead of the usual (and more natural) $M \to \infty$ limit of the Born–Oppenheimer–Heitler–London treatment. The reasoning, made independently by Adamowski et al. [14] and in Ref. [15], is reminiscent of the well-known argument that if an even Hamiltonian, say $h_{\text{even}} = p^2 + x^2$, is supplemented by an odd term $h_{\text{odd}}$, then the ground state is lowered. This is seen explicitly if $h_{\text{odd}} = x$, but the general result follows simply from the variational principle applied to $h_{\text{even}} + h_{\text{odd}}$ using the even ground-state of $h_{\text{even}}$ as trial wave function. Here, parity is replaced by charge conjugation, and the $(M^+, M^+, m^-, m^-)$ Hamiltonian is rewritten as

$$H = H_{\text{even}} + H_{\text{odd}} = \left[\left(\frac{1}{4M} + \frac{1}{4m}\right)(p_1^2 + p_2^2 + p_3^2 + p_4^2) + V\right] + \left[\left(\frac{1}{4M} - \frac{1}{4m}\right)(p_1^2 + p_2^2 - p_3^2 - p_4^2)\right]. \quad (5)$$

The full Hamiltonian $H$ has a lower ground-state than its even part $H_{\text{even}}$, which is nothing but a rescaled version of the $\text{Ps}_2$ case. The nice feature is that $H$ and $H_{\text{even}}$ have the same threshold, since when one computes the two-body energy, one first averages the inverse masses $M^{-1}$ and $m^{-1}$ to calculate the reduced mass.

Once the binding energy of $(M^+, M^+, m^-, m^-)$ is given, then minimal extensions of the stability domain beyond the line $\{m_1 = m_2, m_3 = m_4\}$ can
be derived \[16, 17\].

Many other configurations have been studied in the literature. In particular, all those with \(m_3 = m_4\) have been found to be stable. This property was checked extensively in Ref. \[18\]. Thus, for two identical electrons (\(m_3 = m_4\)), the molecule is always stable, irrespective of whether are the masses of the nuclei are equal or unequal, heavier or lighter than the electrons, or even one lighter and one heavier.

The results obtained can be very conveniently described using the tetrahedron of Fig. 4, which is also referred to by Armour \[19\]. The thick lines correspond to stable configurations with \(\alpha_1 = \alpha_2 = 0\) or \(\alpha_3 = \alpha_4 = 0\). The middle is just the familiar hydrogen molecule with infinitely heavy protons. The thin sides are outside the stability domain. The configuration at the middle of a thin line corresponds to \((p, e^+, \bar{p}, e^-)\), studied in detail in \[19\]. The protonium \((\bar{p}p)\) forms a neutral and compact object with much too small an internuclear separation to bind the positronium atom \((e^+e^-)\).

### 3 Further studies

So far, we have restricted ourselves to the ground state and to unit charge. Several generalizations can be envisaged.

The case of three particles with arbitrary charges \(\pm(q_1, -q_2, -q_3)\) is discussed rather extensively in Refs. \[20, 21\].

In principle, our study can be repeated for excited states. For the first state with specific quantum numbers (negative parity, or a given value of the total angular momentum), the convexity properties remain, as one is dealing with the ground state in another sector of the Hilbert space. For the second or third state of given quantum numbers, the situation is more delicate.

For excited states, stability should be addressed with respect to the appropriate threshold. For instance, a three-charge state of unnatural parity \(J^P = 1^+\) cannot decay into the ground state of an atom and an isolated charge, unless a photon is also emitted. If one neglects radiative processes, then the lowest threshold involves an excited atom and is thus much higher than the threshold relevant for natural-parity states.

The rigorous results on these systems are rather limited. There are fortunately more and more powerful methods which can be used for numerical investigations, among which are the stochastic variational method \[22\] and Monte-Carlo methods \[23\]. Among the remarkable results obtained by
sophisticated numerical methods, we already mentioned the evidence that $(m_1^+, m_2^+, 1^-, 1^-)$ systems are stable $\forall m_1, m_2$. There is also the discovery of stable excited states for the Positronium molecule [24].

Coulomb systems with more than four particles have been investigated. In the case of bosons, say $(m^+, m^-)^N$, it has been known for long-time that the system becomes more and more bound when the number $2N$ of constituent increases. A kind of precocious approach to the large $N$ limit was found in Ref. [25]. More precise binding energies are provided in Ref. [22]. In more recent papers, Varga et al. revealed several new stable configurations with an atom or an ion binding two positrons [26, 27].

The methods can also be applied to other potentials. For power-law potentials, the scaling laws are comparable to those of the Coulomb case, and the stability region can be drawn in a triangle for three-body systems, and a tetrahedron for four bodies, with similar convexity properties. Otherwise, the representation acquires additional dimensions.

The role of the number of space dimensions has also been studied [28].

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