Domain of stability of unnatural parity states of three unit charges

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We investigate the domain of masses for which a bound state with total orbital momentum $L=1$ and unnatural parity $P=+1$ exists for the Coulomb systems (m_1^+, m_2^-, m_3^-).

I. INTRODUCTION

There is an abundant literature on Coulomb systems, in particular, ions made of three unit charges, $(m_1^\pm, m_2^\mp, m_3^\mp)$. For the ground state with total angular momentum and parity $L^P=0^+$, some particular configurations have been studied in great detail, and the map of the stability domain has been drawn, when the masses m_i are varied. For a review, and references, see, e.g., [1].

The study of this 0^+ ground state indicates a number of interesting features. There is a variety of situations: deep binding as for H_2^+, instability as for $(p, \bar{p}, e^-)$, and states at the edge of binding, such as $Ps^-(e^+, e^-, e^-)$ or $H^-(p, e^-, e^-)$. The stability is reinforced when two particles become identical $(m_2 = m_3)$. Schematically, the system has two components: a (m_1^+, m_2^-) cluster with a loosely attached third particle, or (m_1^+, m_3^-) cluster weakly linked to the second particle; when the thresholds become identical, the two components have maximal interference to build a compound system.

Note, however, that for these symmetric systems $(M^\pm, m^\mp, m^\mp)$, the stability, as measured by the dimensionless parameter $r=(E-E_{\text{th}})/E_{th}$ comparing the energy E to the threshold energy E_{th} is *not* a monotonic function of the mass ratio M/m [1]. Its minimum lies between $M/m \gg 1$ (H^-) and $M/m=1$ (Ps^-). It is thus conceivable that an excitation that exists for H^- does not survive for finite M/m.

For a fragile system such as H^-, the Hartree-Fock picture fails. No variational wave function $f(r_{12})f(r_{13})$ gives an expectation value lower than the threshold energy. One needs either a explicit r_{23} dependence in the wave function, or a breaking of factorization, as in the famous Chandrasekhar wave function [2],

$$\Psi = \exp(-ar_{12} - br_{13}) + \exp(-br_{12} - ar_{13}), \quad (1)$$

in which the particle identity is first broken and then restored by a counterterm, a strategy sometimes named "unrestricted Hartree-Fock" [3]. In natural units, the $H(1s)+e^-$ threshold for H^- is at -0.5, the above wave function gives an energy of about -0.513, and the elaborate calculations about -0.528. So it is not surprising that there is only one bound state below this lowest threshold, as rigorously demonstrated by Hill [4].

However, the attention was later paid on the positive-parity state where each electron is a p wave, coupled to form a total angular momentum $L=1$. Such a state with $L^P=1^+$ cannot decay into $H(1s)+e^-$ as long as radiative corrections and spin effects are neglected. Its effective threshold consists of $H(2p)+e^-$, at -0.125. Variational calculations, first at Oslo [5] and confirmed elsewhere (see, e.g., [6,7]), give an energy of about -0.12535, just below the threshold. Grosse and Pittner [8] have shown that this is the only unnatural parity state of H^- with this type of stability. But higher configurations of unnatural parity exist, for instance by attaching a positron to a two-electron system of unnatural parity [9].

Starting from H^- and exchanging the masses leads to H_2^+, whose ground state is deeply bound and excitation spectrum very rich, and not surprisingly, includes a stable 1^+ state. However, Mills [10] investigated the case of equal masses, i.e., Ps^-, and found the 1^+ state to be unbound. More precisely, he studied the 1^+ state for any configuration (M^+, m^-, m^-) and got stability everywhere except for

$$0.059 \lesssim m/M \lesssim 2.36. \quad (2)$$

This estimate was confirmed by Bhatia and Drachman [11]. It is the aim of the present note to check the domain of stability for (M^+, m^-, m^-) found in [10,11] (without trying to challenge their accuracy), and to extend the study to the case of unequal masses for the negative charges. It is organized as follows. In Sec. II, we summarize the rigorous results on the stability domain. The variational method and the results are presented in Sec. III, and Sec. IV is devoted to some conclusions.

II. PROPERTIES OF THE STABILITY DOMAIN

We consider the Hamiltonian

$$H = \frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} + \frac{\mathbf{p}_3^2}{2m_3} - \frac{1}{r_{12}} - \frac{1}{r_{23}} + \frac{1}{r_{23}}, \quad (3)$$

and focus on the lowest $L^P=1^+$ state. The center-of-mass motion can be removed explicitly by introducing Jacobi coordinates, or in the variational calculations, by using trial wave functions that are translation invariant. By scaling, each charge can be set to unity, and one can impose that the inverse masses $\alpha_i = 1/m_i$ obey $\alpha_1 + \alpha_2 + \alpha_3 = 1$. Thus, as done for the 0^+ ground state [1,12], each physical system with $m_i > 0$ can be represented as a point inside an equilateral
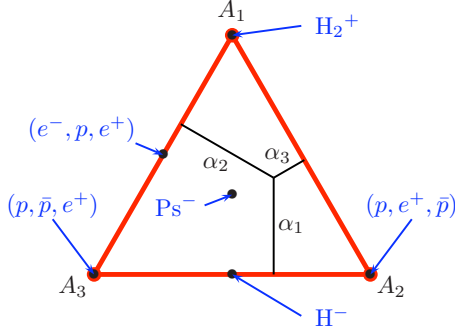
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FIG. 1. (Color online) Representation of a (m_1^+, m_2^+, m_3^+) Coulomb system from its normalized inverse masses $\alpha_i = m_i^{-1}/(m_1^{-1} + m_2^{-1} + m_3^{-1})$. Some special cases are also shown.

triangle, and the inverse masses α_i are proportional to the distances to the sides. See Fig. 1.

In this representation, the frontier between stability and instability has the following properties:

(i) It is symmetric with respect to the vertical axis, due to $2 \leftrightarrow 3$ exchange,

(ii) In each of the half-triangles limited by the symmetry axis, the instability domain is convex.

(iii) The instability domain including, say, the point A_2 with inverse masses $(0,1,0)$ is star shaped with respect to A_2. (A semistraight line starting from A_2 enters at the most once a stability domain until it reaches the symmetry axis.)

(iv) If an energy

$$E = E_{\text{th}}(1 + \epsilon), \tag{4}$$

is found for (M^+, m^-, m^-), where $E_{\text{th}} = -Mm/[2(M+m)]$ is the (M^+, m^-) threshold, and ϵ measures the relative fraction of extra binding, and if one considers an asymmetric combination (m_1^+, m_2^-, m_3^-) with $m_1 = M$ and the same average inverse mass in the negative sector, i.e., $m_1^{-1} + m_2^{-1} = 2m^{-1}$, then stability extends at least up to

$$|m_1^{-1} - m_2^{-1}| = \frac{2\epsilon}{1 + \epsilon}(M^{-1} + m^{-1}). \tag{5}$$

Note that near the symmetry axis, the Hamiltonian $H(m_1, m_2, m_3)$ can be split into a symmetric and an antisymmetric parts,

$$H(m_1, m_2, m_3) = H(m_1, \bar{m}, \bar{m}) + \left(\frac{1}{2m_2} - \frac{1}{2m_3}\right)(\mathbf{p}_2^2 - \mathbf{p}_3^2), \tag{6}$$

with $\bar{m}^{-1} = (m_2^{-1} - m_3^{-1})$. The energy of the three-body system varies at second order in the mass difference, while the threshold energy varies at first order.

The proof of the above results is the same as for the 0^+ ground state [1,12]. However, in this latter case, its was also demonstrated that any configuration with $m_2 = m_3$ has at most one bound state [4], so that the entire stability domain was connected, and clustered near the symmetry axis. This is not the case of $L^P = 1^+$, as no stable state exists for equal masses [10,11]. Hence, the stability domain includes two separate islands, one around H_2^+, and another around H^-.

III. VARIATIONAL METHOD AND RESULTS

A. Trial wave function

For scalar states, a generalization of Eq. (1) is

$$\Psi = \sum_i \gamma_i \exp(-a_i x - b_i y - c_i z), \tag{7}$$

where $\mathbf{x} = \mathbf{r}_{23}, \ldots$ join the particles and $x = |\mathbf{x}|, \ldots$ are the relative distances. After integration over the trivial angular variables, one is left with integrating over $xyz dx dy dz$, submitted to the triangular inequality. The matrix elements can be deduced from the generic function

$$F(\alpha, \beta, \gamma) = \int \int \int_{|x-y| \leq z \leq x+y} \exp(-\alpha x - \beta y - \gamma z) dx dy dz$$

$$= \frac{4}{(\alpha + \beta)(\beta + \gamma)(\gamma + \alpha)}, \tag{8}$$

and its derivatives.

For a $L^P = 1^+$ state with projection $L_3 = j$, a trial function is the superposition

$$\Psi = (\mathbf{y} \times \mathbf{z})_j \sum_i \gamma_i \exp(-a_i x - b_i y - c_i z), \tag{9}$$

with the possibility of enforcing explicitly the $x \leftrightarrow y$ symmetry if $m_2 = m_3$. Once the integration is carried out over the angular variables, one can express, again, all the matrix elements in terms of the derivatives of F. For a given set of range parameters, the weights γ_i are given by a generalized eigenvalue problem. It is possible to assign the a_i, b_i, c_i to have values in a restricted set $(u, v, \ldots)$, i.e., $(a_i, b_i, c_i) = (u, u, u), (u, u, v), \ldots (u, v, w), \ldots (w, w, w), \ldots$, and even assume $(u, v, \ldots)$ in a kind of progression, in order to simplify the minimization over the nonlinear parameters, without a significant loss of accuracy. This is similar to the strategy used, e.g., by Kamimura *et al.* when handling the expansions over Gaussians [13].

B. H⁻-like states

For H⁻, the energy is found to be $E \simeq -0.1253$, as in the literature. For other symmetric configurations (M^+, m^-, m^-), we obtain stability for $M/m \gtrsim 2.39$, in good agreement with Mills's estimate [Eq. (2)]. The width of the stability domain is very narrow. For an infinitely massive proton, we find stability only for $m_3/m_2 \lesssim 1.006$ (if $m_3 \geq m_2$). This is very close to the estimate based on Eq. (5), as expected for such a small width. For instance, the 1^+ state does not exist for the very exotic (p, π^-, μ^-) system.

C. H₂⁺-like states

Stability is found for (M^+, m^-, m^-) with $M/m \lesssim 0.055$, again in good agreement with Eq. (2). On the side of the triangles, we obtain stability for the inverse masses $(1 - \alpha, \alpha, 0)$ and the symmetric points $(1 - \alpha, 0, \alpha)$ for $0 \leq \alpha \lesssim 0.094$. For the point of the symmetry axis with the inverse masses $(1 - \alpha, \alpha/2, \alpha/3)$, the relative excess of energy is
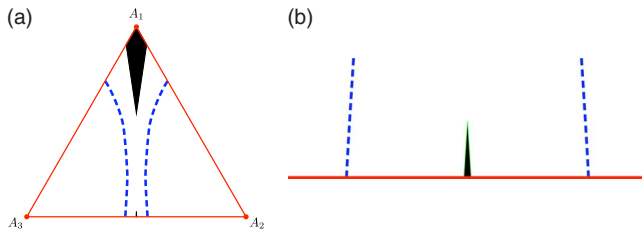
FIG. 2. (Color online) Domain of stability for (m_1^+, m_2^-, m_3^-) in the triangle of normalized inverse masses: the ground state 0^+ (dashed lines) and the unnatural parity state 1^+ (solid). On the right, magnification of the bottom part of the plot.

found to be $\epsilon \simeq 0.034$, and Eq. (5) is underestimates the width of the domain by about 15%.

D. Summary

The domain of stability contains at least the areas displayed in Fig. 2. The frontier is almost straight, so the convexity of the instability domain is weakly pronounced. The spike around H^- is very small and extremely narrow, and shows up only after magnification. For comparison, the domain of stability of the ground state 0^+ is also shown. Due to the convexity and star-shape properties mentioned in Sec. II, isolated islands of stability cannot exist.

IV. OUTLOOK

The case of unnatural parity states of three unit-charge particles displays an interesting—and rare—example of *discontinuous* stability domain, where stability disappears and shows up again, when some constituent masses are varied continuously and monotonously. This means that the transition from a molecular type of binding (H_2^+) to a halo-type of binding (H^-) involves some more fragile intermediate dynamics of stability.

Clearly, for these states at the edge between stability and instability, any minor correction can move the frontier. In particular, it would be interesting to investigate the role of relativistic corrections, which could act slightly differently in the three-body system and in the atom entering the threshold.

The unnatural parity sector plays an important role for other few-body systems, in particular the positronic complexes [9]. In baryon spectroscopy, the unnatural parity states with $J^P = 1^+$ are predicted in the three-quark model but have not yet been seen, and this led to suggest a quark-diquark picture of baryons [14].

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