Few-Body Systems 22, 37–60 (1997)

Few-Body Systems



# Rigid-Rotator and Fixed-Shape Solutions to the Coulomb Three-Body Problem

A. Santander, J. Mahecha, and F. Pérez

Departamento de Física, Universidad de Antioquia, AA 1226, Medellín, Colombia

**Abstract.** Solutions to the general classical Coulomb three-body problem in the form of rigid-rotator and fixed-shape configurations are studied. In the collinear case, some necessary and/or sufficient conditions for the existence of the so-called charge-symmetrical, $(-)(+)(-)$, and charge-asymmetrical, $(-)(-)(+)$, configurations are stated. These conditions involve relations between the geometrical and dynamical parameters of the system under study. The impossibility of the existence of a planar Coulombic rigid rotator is demonstrated. In the two-dimensional case, fixed-shape solutions are studied analytically, and it is shown that, in the three-dimensional case, only fixed-shape solutions involving a triple collision and a static case are possible. Finally, some numerical experimentation, mostly based upon theoretical predictions of the work, is performed, and new bound (although unstable) rotating-oscillating orbits for systems such as the positronium negative ion and helium are found.

## 1 Introduction

The classical three-body problem (three particles with arbitrary masses and charges interacting through gravitational or Coulomb forces) is one of the fundamental, and still not completely explored, problems of mathematical physics. Its study is important in a variety of physics and mathematics fields [6, 9, 23, 31]. It also has a long tradition in connection with chaos research, being the problem that led Poincaré to make his famous remarks concerning the sensitive dependence on the initial conditions exhibited by certain dynamical systems [13].

It was Lagrange who, interested in celestial mechanics, first attacked the problem within the framework of classical dynamics [9]. He formulated the gravitational problem rigorously and found a few particular solvable cases (called “Lagrange’s configurations” [24]). In the realm of atomic physics, the problem is first met when attempting to evaluate the energy spectrum of two-electron atoms – the helium problem.

The general (classical) three-dimensional three-body problem has been studied extensively through numerical simulations [14, 27] and analytical studies [7, 11, 20]. The fact that it is a non-integrable problem [24] makes it too complicated for a systematic analysis in full generality, and has led to the study of various simplifications or restrictions of its geometrical (inter-particle distances) and/or dynamical parameters (masses and charges), which include: the restricted three-body problem; the helium-like problem; the rectilinear three-body problem; the planar gravitational three-body problem; the three-dimensional problem with finite non-zero masses, but with special symmetries; and the three-dimensional rigid-rotator configurations.

In this paper, we intend to study, from a classical point of view, the general Coulomb three-body problem (with arbitrary masses and charges), in the framework of the last four simplifications stated above. Even though the most important applications of such a study would be in atomic and molecular physics (and so, in rigour, quantum mechanics should be applied instead [2, 5, 21, 22]), considerations from classical mechanics may be really useful in various cases, especially concerning states with some “classical character,” such as the highly (doubly) excited states [9, 28]; it should be stressed that for low quantum numbers, in particular the ground state, concepts like classical trajectory and its stability are irrelevant. Besides, it came to the physicist’s attention a few decades ago that some physically relevant values could be extracted from a classical-mechanics analysis through a suitable application of the correspondence principle [25, 26]. Furthermore, the exact quantum computation of certain matrix elements may be cumbersome, or very demanding in terms of numerical accuracy and time, while their corresponding semiclassical evaluation remains tractable [15, 19].

Sect. 2 analyzes the collinear configuration and the planar non-collinear configuration. In Sect. 3, a brief review of the results obtained by some other authors in the study of the three-dimensional rigid configurations and then a detailed study of the general so-called “fixed-shape solutions” are given, and some general conclusions regarding these configurations are drawn. The existence of fixed-shape solutions in rotating collinear configurations and triple-collision motions as well as in static configurations is shown. Sect. 4 contains some numerical results, obtained by integrating the equations of motion. Finally, in Sect. 5, conclusions and some open questions are stated.

## 2 Rigid Collinear Configurations

Rotating rigid solutions in which the particles remain collinear throughout the motion, in the case of two identical negatively charged particles moving along a circle on opposite sides of a third positively charged one, have been studied by several authors [10, 28]. This is a case of the well-known Wannier configurations. The aim of this section is to study the general problem of three interacting charged particles (two negative and one positive) with arbitrary masses and magnitudes of charges, asking if it is possible for the system to move so that the three particles lie always on a line passing through $G$ (the centre of mass of the system), which rotates uniformly in a plane about this point with an angular velocity $\Omega$. Since the Coulomb interaction can be of two types (repulsive or attractive), two different cases can arise: one in which the positive particle is placed between the two negative particles (we shall call this case “charge-symmetrical configuration”), and one in which the two negative particles are adjacent and the positive particle is in one of the extreme positions of the configuration (“charge-asymmetrical configuration”). We shall begin by studying the charge-symmetrical configuration.

### *2.1 Charge-Symmetrical, or (−)(+)(−), Configuration*

Let us denote the three particles by $A_1,\ A_2,\ A_3$, so that each particle has the following masses and charges,

$$\begin{aligned} A_1&: \quad m_1, -Z_1 e,\\ A_2&: \quad m_2, +Z_2 e,\\ A_3&: \quad m_3, -Z_3 e, \end{aligned} \tag{1}$$

where $e > 0$ is an arbitrary charge unit, and all $m_i$ and $Z_i$ ($i$ = 1, 2, 3) are positive numbers (see Fig. 1 a). For simplicity, we set the constant of the Coulomb interaction equal to one.

Let now the distances from $G$, measured in the same direction, be $x_1, x_2, x_3$. We may assume, without loss of generality, that $x_1 < x_2 < x_3$, so $x_1 < 0$ and $x_3 > 0$. Then, if $\Omega$ is the angular velocity of the system, Newton's second law requires:

$$m_1\Omega^2 x_1 = -\frac{Z_1 Z_2}{(x_2 - x_1)^2} e^2 + \frac{Z_1 Z_3}{(x_3 - x_1)^2} e^2, \tag{2}$$

$$m_2\Omega^2 x_2 = \frac{Z_1 Z_2}{(x_1 - x_2)^2} e^2 - \frac{Z_3 Z_2}{(x_3 - x_2)^2} e^2, \tag{3}$$

$$m_3\Omega^2 x_3 = \frac{Z_2 Z_3}{(x_2 - x_3)^2} e^2 - \frac{Z_1 Z_3}{(x_1 - x_3)^2} e^2. \tag{4}$$

It should be noticed that Eq. (3) is valid whether $x_2$ is positive or negative.

Let us introduce the inter-particle distances as: $r_1 = x_3 - x_2$, $r_2 = x_3 - x_1$, and $r_3 = x_2 - x_1$. We now look for fixed values for the ratios $r_1 : r_2 : r_3$. If we define

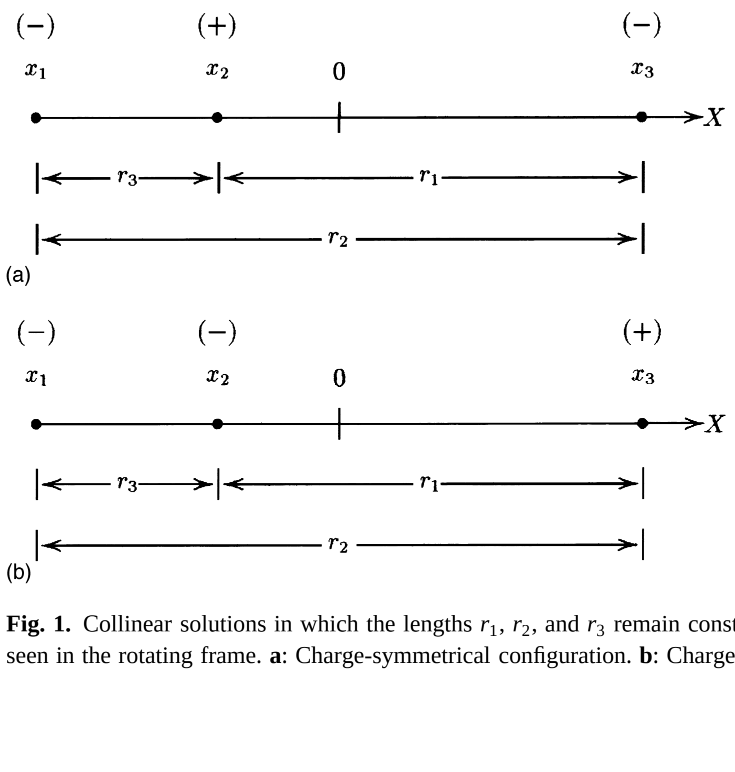


**Fig. 1.** Collinear solutions in which the lengths $r_1$, $r_2$, and $r_3$ remain constant throughout the motion, as seen in the rotating frame. **a**: Charge-symmetrical configuration. **b**: Charge-asymmetrical configuration

$k \equiv r_1/r_3$ so that

$$\frac{r_1}{k} = \frac{r_2}{k+1} = \frac{r_3}{1}, \tag{5}$$

we have

$$k = \frac{x_3 - x_2}{x_2 - x_1}. \tag{6}$$

Evaluating $x_3 - x_2$ and $x_2 - x_1$ from Eqs. (2)–(4), and substituting the result into expression (6), we obtain the following 5th-order equation for $k$,

$$\frac{Z_1Z_2}{\mu_{12}}k^5 + Z_1Z_2\left(\frac{2}{m_1}+\frac{3}{m_2}\right)k^4 + \left[Z_1Z_2\left(\frac{1}{m_1}+\frac{3}{m_2}\right) - \left(\frac{Z_1Z_3}{m_1}+\frac{Z_2Z_3}{m_2}\right)\right]k^3$$
$$+\left[\left(\frac{Z_1Z_3}{m_3}+\frac{Z_1Z_2}{m_2}\right) - Z_2Z_3\left(\frac{3}{m_2}+\frac{1}{m_3}\right)\right]k^2 - Z_2Z_3\left(\frac{3}{m_2}+\frac{2}{m_3}\right)k - \frac{Z_2Z_3}{\mu_{23}} = 0, \tag{7}$$

where $\mu_{ij} = m_i m_j/(m_i + m_j)$, with $i, j$ = 1, 2, 3.

### 2.1.1 Existence of Solutions

The physically meaningful solutions to our problem will be related to the positive real roots of the above equation. In order to look for such roots, we use Descartes' signs rule [3], by first observing that the coefficients of $k^5$ and $k^4$ are always positive, and the coefficients of $k^1$ and $k^0$ negative. Then, if we call $C_i$ the coefficient of $k^i$ ($i = 0, \ldots, 5$), we have the following nine different possibilities for the number of positive real roots of Eq. (7):

a) $C_3 > 0$ and $C_2 > 0$. One.
b) $C_3 > 0$ and $C_2 < 0$. One.
c) $C_3 < 0$ and $C_2 > 0$. Three or one.
d) $C_3 < 0$ and $C_2 < 0$. One.
e) $C_3 = 0$ and $C_2 > 0$. One.
f) $C_3 = 0$ and $C_2 < 0$. One.
g) $C_3 > 0$ and $C_2 = 0$. One.
h) $C_3 < 0$ and $C_2 = 0$. One.
i) $C_3 = 0$ and $C_2 = 0$. One.

In conclusion, for all the cases, there is always at least one physically meaningful value for $k$. This fact, however, is still not an answer to the question regarding the existence of solutions to the (−)(+)(−) configuration, as we shall see next.

From Eqs. (2)–(4), and the definitions of $r_i$ ($i$ = 1, 2, 3) and $k$, we can deduce

$$\Omega^2 = \frac{e^2}{r_3^3}\left\{\frac{1}{m_3}\,\frac{Z_2Z_3}{k^2(k+1)} + \frac{1}{m_1}\,\frac{Z_1Z_2}{k+1} - \frac{1}{\mu_{13}}\,\frac{Z_1Z_3}{(k+1)^3}\right\}, \tag{8}$$

which, in order to have a positive value for $\Omega^2$, poses a restriction on the domain available to $k$, namely

$$(k+1)^2\left[\frac{Z_2Z_3}{m_3} + \frac{Z_1Z_2}{m_1}k^2\right] \geq \frac{Z_1Z_3}{\mu_{13}}. \tag{9}$$

In this fashion, we conclude that if the collinear charge-symmetrical configuration (−)(+)(−) actually exists (so that $k > 0$ and $\Omega^2 > 0$), then $k$ must fulfill condition (9), and conversely, if $k$ obeys Eq. (9), the configuration (−)(+)(−) exists for all possible cases.

### *2.2 Charge-Asymmetrical, or (−)(−)(+), Configuration*

Let us perform the following changes in notation:

$$\begin{aligned} A_1&: \quad m_1, -Z_1 e,\\ A_2&: \quad m_2, -Z_2 e,\\ A_3&: \quad m_3, +Z_3 e. \end{aligned} \tag{10}$$

Here, again, $x_1, x_2$, and $x_3$ are the distances from $G$ measured in the same direction as in the symmetrical configuration (see Fig. 1 b).

It can be verified that, in this case, the equations of motion are equivalent to those of the previous configuration, (−)(+)(−), if we perform the changes $Z_2 \longrightarrow -Z_2$ and $Z_3 \longrightarrow -Z_3$. Taking this into account, and retaining the definitions for $r_i$ ($i$ = 1, 2, 3) and $k$, the equation for $k$ becomes:

$$\begin{aligned} &-\frac{Z_1Z_2}{\mu_{12}}k^5 - Z_1Z_2\left(\frac{2}{m_1}+\frac{3}{m_2}\right)k^4 + \left[-Z_1Z_2\left(\frac{1}{m_1}+\frac{3}{m_2}\right)+\left(\frac{Z_1Z_3}{m_1}-\frac{Z_2Z_3}{m_2}\right)\right]k^3\\ &\qquad -\left[\left(\frac{Z_1Z_3}{m_3}+\frac{Z_1Z_2}{m_2}\right)+Z_2Z_3\left(\frac{3}{m_2}+\frac{1}{m_3}\right)\right]k^2 - Z_2Z_3\left(\frac{3}{m_2}+\frac{2}{m_3}\right)k - \frac{Z_2Z_3}{\mu_{23}} = 0. \end{aligned} \tag{11}$$

It must be noted that the coefficients of $k^i$ ($i = 0, 1, 2, 4, 5$) are now always negative. Therefore, only three different cases arise:

a) $C_3 > 0$. Two or zero positive real roots.
b) $C_3 < 0$. No positive real roots.
c) $C_3 = 0$. No positive real roots.

#### 2.2.1 Necessary Conditions for the Existence of a Solution

From the analysis given above, we conclude that only if

$$\frac{Z_1Z_3}{m_1} > \frac{Z_2Z_3}{m_2} + Z_1Z_2\left(\frac{1}{m_1}+\frac{3}{m_2}\right), \tag{12}$$

then the collinear (−)(−)(+) configuration might be possible. However, this is not a sufficient condition for the existence of such a configuration (because, in some special cases, the number of positive real roots could be zero, or the positive real roots could not satisfy the condition (14) stated below). In particular, condition (12) is not satisfied by a system in which $Z_1 = Z_2$ and $m_1 = m_2$.

On the other hand, if such a configuration existed (and so $k \in \{k_1, k_2\}$), the two possible angular velocities of the system would be given by

$$\Omega_i^2 = \frac{e^2}{r_3^3}\left\{\frac{1}{m_3}\,\frac{Z_2Z_3}{k_i^2(k_i+1)} - \frac{1}{m_1}\,\frac{Z_1Z_2}{k_i+1} + \frac{1}{\mu_{13}}\,\frac{Z_1Z_3}{(k_i+1)^3}\right\} \qquad (i = 1, 2) \tag{13}$$

and the allowed domain for $k_i$ ($i = 1, 2$) would be determined from

$$\left(k_i + 1\right)^2 \left[\frac{Z_2 Z_3}{m_3} - \frac{Z_1 Z_2}{m_1} k_i^2\right] \geq -\frac{Z_1 Z_3}{\mu_{13}}. \tag{14}$$

We may now conclude that if two positive roots of Eq. (11), $k_1$ and $k_2$, can be found, then the configuration $(-)(-)(+)$ exists if and only if one or both of such $k_i$ belong to the domain given by condition (14). Below we shall show an explicit example of the existence of these solutions.

### *2.3 Impossibility of a Plane Rigid Two-Dimensional Rotator*

Following the reasonings given in ref. [24] for the gravitational case, we have proved the non-existence of a rigid two-dimensional configuration of the Coulombic rotator. For the case of a system with two identical negatively charged particles, this had already been stated as an intuitive fact by Grujić [9].

The notation to be used is the same as in the problem of the $(-)(-)(+)$ configuration, and we shall refer in some of the reasonings to Figs. 2 a and b.

Let us start from the assumption that such a configuration does in fact exist. Then, the particle $A_3$ must verify the equilibrium conditions

$$\frac{Z_1}{r_2^2} \sin\theta_2 = \frac{Z_2}{r_1^2} \sin\theta_1, \tag{15}$$

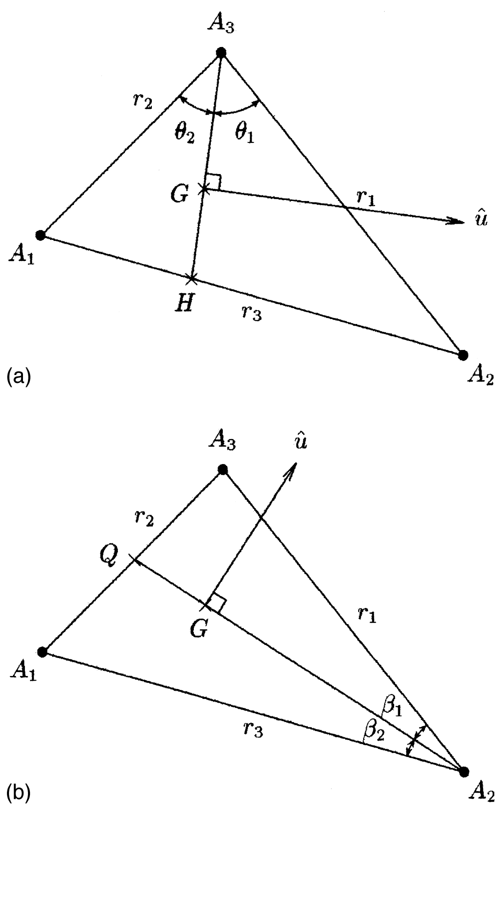


**Fig. 2.** Diagrams used in the proof of the inexistence of a rigid two-dimensional rotator. $G$ is centre of mass of the system, $Q$ the one of particles $A_1$ and $A_3$, and $H$ the one of particles $A_1$ and $A_2$

$$\frac{m_3}{Z_3 e^2}\,\Omega^2\overline{A_3G} = \frac{Z_1}{r_2^2}\cos\theta_2 + \frac{Z_2}{r_1^2}\cos\theta_1, \tag{16}$$

with $\theta_1 = \angle\big(HA_3A_2\big)$, $\theta_2 = \angle\big(A_1A_3H\big)$, $\theta_1$ and $\theta_2 \in [0, \pi]$, and $H$ the centre of mass of $A_1$ and $A_2$ (see Fig. 2 a). Now, from the geometry of the triangle $A_1A_2A_3$ and the equation that defines the position of $H$, $m_1\overline{A_1H} = m_2\overline{HA_2}$, we deduce

$$\frac{r_1 \sin\theta_1}{r_2 \sin\theta_2} = \frac{\overline{HA_2}}{\overline{A_1H}} = \frac{m_1}{m_2}. \tag{17}$$

In this way, from Eqs. (15) and (17), we finally have the ratio:

$$\frac{r_1}{r_2} = \left(\frac{m_1Z_2}{m_2Z_1}\right)^{1/3}. \tag{18}$$

On the other hand, the dynamics of particle $A_2$ yields (see Fig. 2 b)

$$\frac{Z_3}{r_1^2}\sin\beta_1 = -\frac{Z_1}{r_3^2}\sin\beta_2, \tag{19}$$

$$\frac{m_2}{Z_2e^2}\,\omega^2 A_2G = \frac{Z_3}{r_1^2}\cos\beta_1 - \frac{Z_1}{r_3^2}\cos\beta_2, \tag{20}$$

with $\beta_1 = \angle\big(A_3A_2Q\big)$, $\beta_2 = \angle\big(QA_2A_1\big)$, $\beta_1$ and $\beta_2 \in [0, \pi]$, and $Q$ the centre of mass of $A_1$ and $A_3$. Finally, from the geometry of Fig. 2 b, we have

$$\frac{\sin\beta_1}{\sin\beta_2} = \frac{m_3r_1}{m_1r_3}. \tag{21}$$

Combining Eqs. (19) and (21), we find

$$\frac{r_1}{r_3} = -\left(\frac{Z_1m_3}{Z_3m_1}\right)^{1/3}. \tag{22}$$

And, by analogous calculations on particle $A_1$,

$$\frac{r_2}{r_3} = -\left(\frac{Z_2m_3}{Z_3m_2}\right)^{1/3}. \tag{23}$$

From Eqs. (18), (22), and (23), and the fact that, by definition, $r_i > 0$, $Z_i > 0$, $m_i > 0$ ($i = 1, 2, 3$), we arrive immediately at a contradiction (note the minus sign in Eqs. (22) and (23)). Thus, we have proven that for the general Coulomb three-body problem it is impossible to obtain a plane rigid-rotator non-collinear solution.

This result could have been deduced also from Eq. (19), due to the minus sign present in this equation and the fact that $\beta_1, \beta_2 \in [0, \pi]$. Note also that this result is still valid if $G$ is no longer the centre of mass of the system, but its centre of charge (or another centre assumed at rest), because the origin of the contradiction is purely dynamical (Eq. (19)) and not geometrical (Eqs. (17) and (21)).

## 3 Fixed-Shape Solutions

We now intend to look for solutions in which the shape of the triangle or the line formed by the three particles is invariant as time evolves, so that the ratios of the inter-particle distances remain constant while the figure oscillates about a given rigid-rotator solution. This kind of solution has been found for the general (planar) gravitational three-body problem [4, 24] and for Coulomb three-body systems [32].

To begin, we shall deal with the three-dimensional case, in which the triangle formed by the particles rotates about an axis through its centre of mass, the orbits of the particles lying in different planes; the plane motion will then be obtained as a particular configuration. The notation and mathematical formalism to be used here will be the same introduced by Grujić and Simonović [10]. A more detailed study of some particular cases of this configuration – including stability analyses – can be found in the papers by Poirier [28] and the afore-mentioned authors, and in references given therein.

### *3.1 Basic Formalism and Introduction of the "Stretching" Function*

Newton's equations for this system read ($i, j = 1, 2, 3$)

$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = \sum_{j \neq i} \varphi_{ij} \mathbf{r}_{ij}, \tag{24}$$

with inter-particle potential functions of the form

$$\varphi_{ij} = \frac{C_{ij}}{r_{ij}^3}, \tag{25}$$

where $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$.

Eq. (24) can be written in a compact form by expressing $\mathbf{r}_3$ as function of $\mathbf{r}_1$ and $\mathbf{r}_2$ in the centre-of-mass frame and introducing coordinates relative to particle 3. This yields (24) the form

$$\mathbf{M} \frac{d^2\mathbf{R}}{dt^2} = \mathbf{\Phi R}, \tag{26}$$

with the definitions

$$\mathbf{M} = \begin{bmatrix} \mu_{12} + \mu_{13} & -\mu_{12} \\ -\mu_{12} & \mu_{12} + \mu_{23} \end{bmatrix}, \tag{27}$$

$$\mu_{ij} = \frac{m_i m_j}{m}, \tag{28}$$

$$m = m_1 + m_2 + m_3, \tag{29}$$

$$\mathbf{R}(t) = \begin{bmatrix} \mathbf{r}_{13} \\ \mathbf{r}_{23} \end{bmatrix}, \tag{30}$$

and

$$\mathbf{\Phi} = \begin{bmatrix} \varphi_{12} + \varphi_{13} & -\varphi_{12} \\ -\varphi_{12} & \varphi_{12} + \varphi_{23} \end{bmatrix}. \tag{31}$$

The most general fixed shape solution can be obtained by a rotation and a homogeneous scale change applied to a constant vector. Assuming that each particle rotates about the $Z$ axis, solutions to the system (26) are sought (as is done, for example, in ref. [10]) in the form of the sum

$$\mathbf{r}_{ij}(t) = \mathbf{f}_{ij}(t;\Omega) + \mathbf{w}_{ij}(t;\Omega), \tag{32}$$

with $\mathbf{f}_{ij}(t;\Omega)$ a vector parallel to the $Z$ axis, and $\mathbf{w}_{ij}(t;\Omega)$ a rotating vector in the $XY$ plane. $\Omega$ is a parameter to be determined later.

It is convenient to write $\mathbf{f}_{ij}$ and $\mathbf{w}_{ij}$ in the form

$$\mathbf{f}_{ij}(t;\Omega) = s(t;\Omega)\mathbf{f}_{ij}(\Omega), \tag{33}$$

$$\mathbf{w}_{ij}(t;\Omega) = g(t;\Omega)\mathbf{w}_{ij}(\Omega), \tag{34}$$

where the "stretching" function $g(t;\Omega)$ is defined by

$$g(t;\Omega) = s(t;\Omega)\exp\{i[\Omega t + b(t;\Omega)]\}, \tag{35}$$

with $s(t;\Omega) = \left|g(t;\Omega)\right|$.

The complex character of $g$ is, of course, a mathematical artifice; it serves to represent by a single number the phase and scaling of $\mathbf{w}_{ij}(t;\Omega)$ with respect to $\mathbf{w}_{ij}(\Omega)$. It makes no sense to multiply the vertical component of Eq. (33) by a complex number.

### 3.1.1 Fixed-Size Solutions

Let us suppose that we have already found a rigid-rotator solution to Eq. (26), described as follows. The asymmetric rotator is a three-dimensional case, in which the triangle formed by the particles rotates about an axis through its centre of mass, the orbits of the particles lying on different planes. A more detailed study of some particular cases of this configuration – including stability analyses – can be found in refs. [10] and [28], and in references given therein.

Since all inter-particle distances are kept fixed, the basic differential system (26) is linear with time-independent coefficients. Its general solution is a linear combination of exponentials. The structure of system (26) ensures that the components of $\mathbf{R}$ are coupled two by two ($\widehat{\mathbf{u}}$ being any of the three fixed rectangular axes, $\mathbf{r}_{13}\cdot\widehat{\mathbf{u}}$ is only coupled to $\mathbf{r}_{23}\cdot\widehat{\mathbf{u}}$). This system is simpler than true solid-motion equations, where the various angular motions are coupled.

A rigid solution has the form given by Eq. (32) with a stretching function $g(t;\Omega) = s_0\exp(i\Omega t)$. In fact, if we define $\mathbf{R} = \mathbf{F} + \mathbf{W}$, whose components are given by Eq. (30) and separated in concordance with definition (32), then Eq. (26) becomes

$$-\Omega^2\mathbf{MW} = \mathbf{\Phi}(\mathbf{F} + \mathbf{W}). \tag{36}$$

Considering that $\mathbf{F}$ and $\mathbf{\Phi}$ are time-independent, Eq. (36) is satisfied if

$$\mathbf{\Phi F} = 0 \tag{37}$$

and

$$-\Omega^2\mathbf{MW}_0 = \mathbf{\Phi W}_0, \tag{38}$$

where it was supposed that $\mathbf{W} = \mathbf{W}_0 \exp(i\Omega t)$. Eq. (37) yields the two-dimensional case, if $\mathbf{F} = \mathbf{0}$, or one of the three-dimensional configurations found by Langmuir and Poirier, if $\mathbf{F} \neq \mathbf{0}$. Note that a non-zero $\mathbf{F}$ requires that $D = \det \boldsymbol{\Phi} = 0$, where $D$ is defined in Eq. (42).

On the other hand, in the rotating term, the time-independent factor $\mathbf{W}_0$ must satisfy

$$\boldsymbol{\Lambda}\mathbf{W}_0(\Omega) = \mathbf{0}, \tag{39}$$

$$\boldsymbol{\Lambda} = \begin{bmatrix} \mathbf{M}_{11}\Omega^2 + \boldsymbol{\Phi}_{11} & \mathbf{M}_{12}\Omega^2 + \boldsymbol{\Phi}_{12} \\ \mathbf{M}_{12}\Omega^2 + \boldsymbol{\Phi}_{12} & \mathbf{M}_{22}\Omega^2 + \boldsymbol{\Phi}_{22} \end{bmatrix}. \tag{40}$$

The secular equation for the angular frequency yields

$$\Omega^2 = \frac{-B \pm (B^2 - 4AD)^{1/2}}{2A} \equiv \Omega'^2, \Omega''^2, \tag{41}$$

with

$$\begin{aligned} A &= \frac{m_1 m_2 m_3}{m}, \\ B &= (\mu_{13} + \mu_{23})\varphi_{12} + (\mu_{12} + \mu_{23})\varphi_{13} + (\mu_{12} + \mu_{13})\varphi_{23}, \\ D &= \varphi_{12}\varphi_{13} + \varphi_{12}\varphi_{23} + \varphi_{13}\varphi_{23}. \end{aligned} \tag{42}$$

As mentioned before, if $D = 0$, the three-dimensional solutions can exist but, if $D \neq 0$, then $\mathbf{F} = \mathbf{0}$ and only a plane case is possible.

It is useful to note that Eqs. (41) and (42) provide us with a first tool to check if a given system of masses and charges can conform to a given rigid-rotator configuration. It suffices to verify that the chosen system yields a real non-negative value for $\Omega^2$.

Two cases arising from Eq. (41) can be distinguished:

(a) $D \neq 0$ (called the "non-degenerate" solution): It can be shown for a system with identical particles 1 and 2 ($\mu_{13} = \mu_{23}$, $C_{13} = C_{23}$) that a so-called Wannier configuration (collinear symmetric rotator, with inter-particle distances equal and opposite) arises (see, for example, ref. [28]).

(b) $D = 0$ ("degenerate" solution): In this case, the relative vectors have two orthogonal components, one constant and the other rotating. There are two values for $\Omega$,

$$\Omega = 0 \qquad \text{and} \qquad \Omega = -\frac{B}{A}. \tag{43}$$

If $\Omega \neq 0$, two cases appear, depending on whether $\varphi_{13} = \varphi_{23}$ or $\varphi_{13} \neq \varphi_{23}$. These are the Langmuir and Poirier cases considered in ref. [10] (see Fig. 3).

The studies performed by the authors of ref. [10] (and by Klar [16, 17]) demonstrate the existence of solutions in the form of a Coulombic rigid three-dimensional rotator with arbitrary values of the masses and charges.

If $\Omega = 0$, we observed a case not discussed in the literature. It is a non-rotating equilibrium configuration corresponding to the symmetric situation illustrated in Fig. 1 a. In order for this solution to exist it is necessary that

$$Z_1 > Z_2 \qquad \text{and} \qquad Z_3 = \frac{Z_1 Z_2}{(Z_1^{1/2} - Z_2^{1/2})^2}. \tag{44}$$

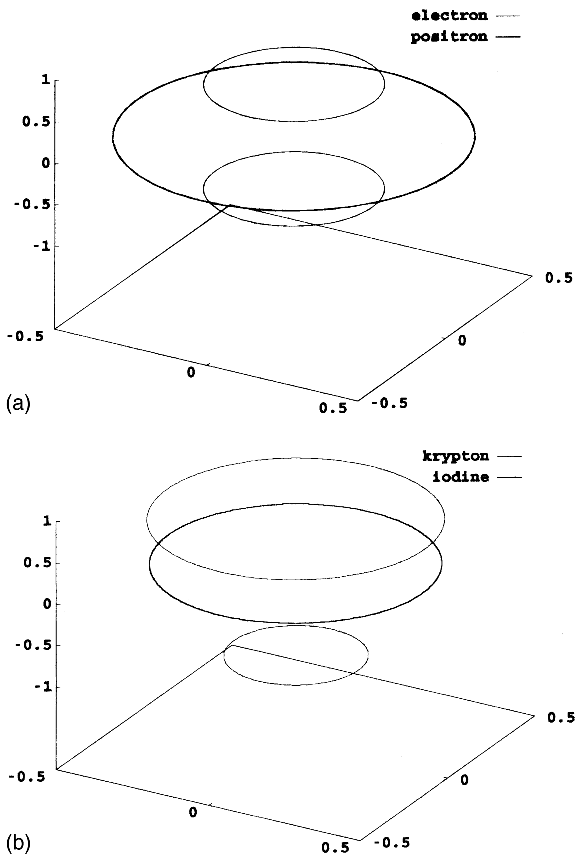


**Fig. 3.** Three-dimensional solution in which the size and shape remain constant throughout the motion. **a**: Langmuir top of the $Ps^{-}$. **b**: Poirier top of $I^{2-} + 2Kr^{3+}$

The overall size of the system is arbitrary and the inter-particle distance ratios are mass-independent and given by

$$k = \frac{Z_2^{1/2}}{Z_1^{1/2} - Z_2^{1/2}}, \tag{45}$$

where $k$ is defined by Eq. (5). Note that this result is compatible with Eqs. (7) and (8), and that no analogous situation in the asymmetric configuration exists. A possible realization of this static equilibrium would be observed in a system constituted by an electron and two beryllium nuclei, as can be obtained from the Diophantine equation in (44).

#### 3.1.2 Non-Fixed-Size Solutions

We now want to study the conditions under which a solution of the form given by Eq. (32) exists, together with definitions (33), (34), and (35). The function $g(t;\Omega)$ "stretches" in a physically suitable fashion each side of the rigid rotating triangle as time evolves, keeping constant the inter-particle distance ratios.

### *3.2 Equation for the Stretching Function*

Now, the solutions to the inter-particle distances (see Eqs. (33) and (34)) were *a priori* chosen to be the product of one particular rigid-rotator solution (see ref. [10]) and a stretching function. It should then be clear that we need only to derive relations between the stretching function and the rest of the system's characteristics.

By replacing the ansatz given in Eqs. (33)–(35), and the substitution $\mathbf{R} = s\mathbf{F} + g\mathbf{W}$, in the matrix Eq. (26) we readily obtain

$$\left[\ddot{s}\mathbf{M} - \frac{1}{s^2}\mathbf{\Phi}(\Omega)\right]\mathbf{F} = 0 \tag{46}$$

and

$$\left[\ddot{g}\mathbf{M} - \frac{g}{s^3}\mathbf{\Phi}(\Omega)\right]\mathbf{W} = 0. \tag{47}$$

This result was found by observing that, if $\mathbf{\Phi}(\Omega)$ represents the matrix of potentials when the inter-particle distances are kept fixed (rigid-rotator configuration), then the matrix $\mathbf{\Phi}$ corresponding to the fixed-shape solutions and the matrix $\mathbf{\Phi}(\Omega)$ are related by

$$\mathbf{\Phi} = \frac{1}{s^3}\mathbf{\Phi}(\Omega). \tag{48}$$

If $\mathbf{W}$ is such that $-\Omega^2\mathbf{MW} = \mathbf{\Phi}(\Omega)\mathbf{W}$, according to Eq. (38), then, using the fact that $\mathbf{MW} \neq \mathbf{0}$, we obtain that $g$ satisfies the same equation of a particle attracted by a fixed centre through a $1/r^2$ force:

$$\ddot{g} = -\Omega^2 \frac{g}{s^3}. \tag{49}$$

We shall write a bound solution to Eq. (49), in the form

$$x_k \equiv \mathrm{Re}(g) = a(1 - e\cos u) \qquad \text{and} \qquad y_k \equiv \mathrm{Im}(g) = a\left(1 - e^2\right)^{1/2} \sin u, \tag{50}$$

where $u$ is the excentric anomaly that satisfies the Kepler equation, $(t - t_0)n\Omega = u - e\sin u$; $n$ is the frequency, $a$ is the larger semi-axis of the ellipse and $e$ is its excentricity. This indicates that the three particles can move following any Kepler orbit. A more general solution is obtained by performing a rotation of the vector $(x_k, y_k)$ (see Figs. 4 d and 6 a). Also unbound fixed-shape solutions exist.

From these relations, we then conclude that, for the fixed-shape solutions, the $XY$ projection of the motion must be given by

$$\begin{aligned}\mathbf{w}_{ij}^f(t) = {} & a\left[x_{ij}(\Omega)(1 - e\cos u) - y_{ij}(\Omega)\left(1 - e^2\right)^{1/2}\sin u\right]\mathbf{e}_x \\ & + a\left[y_{ij}(\Omega)(1 - e\cos u) + x_{ij}(\Omega)\left(1 - e^2\right)^{1/2}\sin u\right]\mathbf{e}_y,\end{aligned} \tag{51}$$

where $x_{ij}(\Omega)$ and $y_{ij}(\Omega)$ correspond to particular initial values of a given rigid-rotator configuration. If $\mathbf{F} = \mathbf{0}$ then Eq. (46) is automatically satisfied, what proves that fixed-shape solutions in which particles move around Kepler-like orbits in a plane always exist.

Now, let us examine the existence of three-dimensional, or $\mathbf{F} \neq \mathbf{0}$, fixed-shape solutions in some special cases. It can be shown that $s = (x_k^2 + y_k^2)^{1/2} = a(1 - e\cos u)$. Then Eq. (46) becomes

$$\left(e\frac{\cos u - e}{1 - e\cos u}\mathbf{M} - \mathbf{\Phi}\right)\mathbf{F} = \mathbf{0}. \tag{52}$$

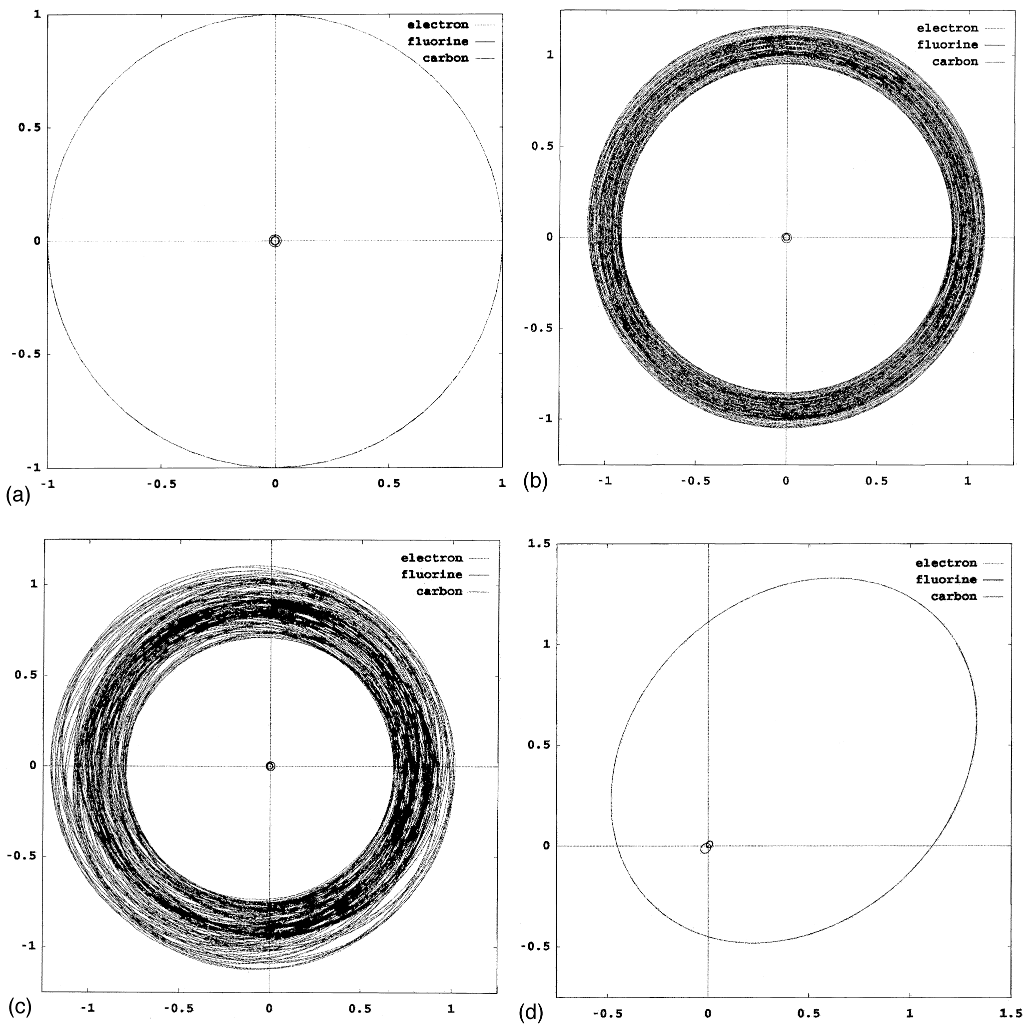


**Fig. 4.** Motions of $e^- + F^- + C^{6+}$ related to the rigid charge-asymmetric configuration. Note the small orbits of the $F^-$ and $C^{6+}$ particles around the origin of coordinates. **a**: Collinear asymmetric configuration. **b**: Variation of $10^2$ on the radial momentum of particle 2. **c**: Variation of $10^2$ on the tangential momentum of particle 2. **d**: Asymmetric fixed-shape solution

Eq. (52) shows that, if $e = 0$, a rigid three-dimensional solution exists, if $\mathbf{\Phi F} = 0$, the same result as given by Eq. (37). Since $u$ is not constant and $\det \mathbf{M} \neq 0$, another possible solution is obtained if $e = 1$, the triple-collision solution. Relativity, however, precludes triple, as well as binary, collisions. The maximal excentricity of the binary collision with Coulombic forces is given in terms of the frequency of the Kepler motion $n$, the larger semiaxis $a$ and the light velocity $c$ by $e \approx 1 - 2(an/c)^2 \approx 1 - 2(Z\alpha)^2$.

If $\Omega = 0$ and $\mathbf{\Phi F} = 0$, another solution is obtained, namely $\ddot{g} = 0$; this means that $g$ is a linear function of time. Considering that in the static case the size of the system can be arbitrary, then the constant-velocity solution is compatible with the static configuration described in Subsection 3.1.1.

### *3.3 Fixed-Shape Solutions in the Collinear Configuration*

As seen in the last section, general three-dimensional fixed-shape solutions cannot exist, due to the requirement, imposed by the equations of motion, that the $Z$ components of the inter-particle distances must vary with time at a different ratio than the $X$ and $Y$ components do. This fact, however, is itself a proof of the existence of fixed-shape solutions in the two-dimensional case (and, more specifically, in the collinear configurations, because of the impossibility of having a planar non-collinear rigid solution). In this fashion, making $Z = 0$ the plane on which the three particles lie, we obtain for the inter-particle vectors

$$\mathbf{r}_{ij} = \left(x^o_{ij} x_k - y^o_{ij} y_k\right)\mathbf{e}_x + \left(y^o_{ij} x_k - x^o_{ij} y_k\right)\mathbf{e}_y, \tag{53}$$

where $x_k$ and $y_k$ are given by Eq. (50). This indicates that the three particles move along Kepler orbits. It should be observed that this solution is completely general, regardless of the values of the geometrical or dynamical parameters of the system. This result is the generalization to Coulombic forces of that obtained by Lagrange in the gravitational case [24], and the symmetric case is a kind of non-rigid Wannier-type solution.

## 4 Numerical Work

In order to perform numerical studies on the different configurations hereto described, we developed a program that integrates the equations of motion for the general Coulomb three-body problem with arbitrary charges and masses in three-dimensional space [27]. In this section we will briefly outline the mathematical procedure necessary to reliably perform the numerical integration and the resulting program.

### *4.1 Regularization Procedure*

The three-body Hamiltonian presents numerical difficulties whenever any of the inter-particle distances becomes very small because of the singularity of the Coulomb force between two point charges in contact. One standard way of avoiding the problems associated with *binary* collisions (the three-particle collision cannot be regularized) was developed by Aarseth and Zare [1] based on previous work by Kustaanheimo and Steifel [18]. We will omit here the details of the procedure, which is described in full length in ref. [1] and more concisely – for the two-dimensional case – in ref. [30]; only the main expressions will be presented.

After writing the three-body Hamiltonian in the centre-of-mass reference frame with the coordinates relative to $m_3$ defined in Eq. (30), and their conjugate momenta, these are replaced by the so-called regularized coordinates $(Q_j, P_j)$ with $j = 1, 2, \ldots, 8$.

Briefly, we define the canonic sets $(q_i, p_i)$ with $i = 1, 2, \ldots, 6$ in terms of the twelve components of $\{\mathbf{r}_{13}, \mathbf{r}_{23}, \mathbf{p}_1, \mathbf{p}_2\}$. We next expand the dimension of the phase space by renaming variables according to

$$q_r \longrightarrow q_{r+1}, \qquad p_r \longrightarrow p_{r+1} \qquad (r = 4, 5, 6), \tag{54}$$

leaving the variables with $r \leq 3$ as before and defining the mock coordinates and momenta

$$q_4 \equiv 0, \qquad q_8 \equiv 0, \qquad p_4 \equiv 0, \qquad p_8 \equiv 0. \tag{55}$$

Then, the regularized coordinates are defined by

$$\begin{aligned} Q_1 &= \left[\frac{1}{2}\left(\left|\mathbf{r}_{13}\right| + q_1\right)\right]^{1/2}, \\ Q_2 &= \frac{q_2}{2Q_1}, \\ Q_3 &= \frac{q_3}{2Q_1}, \\ Q_4 &= 0, \end{aligned} \tag{56}$$

for $q_1 \geq 0$ or

$$\begin{aligned} Q_2 &= \left[\frac{1}{2}\left(\left|\mathbf{r}_{13}\right| - q_1\right)\right]^{1/2}, \\ Q_1 &= \frac{q_2}{2Q_1}, \\ Q_3 &= 0, \\ Q_4 &= \frac{q_3}{2Q_2}, \end{aligned} \tag{57}$$

for $q_1 < 0$. For the variables $(Q_5, Q_6, Q_7, Q_8)$ we have analogous expressions, simply adding 4 to all indices and replacing $\mathbf{r}_{13}$ by $\mathbf{r}_{23}$.

Now, if we define the matrices $\mathbf{A}_1$ and $\mathbf{A}_2$ by

$$\mathbf{A}_1 = 2\begin{bmatrix} Q_1 & Q_2 & Q_3 & 0 \\ -Q_2 & Q_1 & Q_4 & 0 \\ -Q_3 & -Q_4 & Q_1 & 0 \\ Q_4 & -Q_3 & Q_2 & 0 \end{bmatrix}, \tag{58}$$

$$\mathbf{A}_2 = 2\begin{bmatrix} Q_5 & Q_6 & Q_7 & 0 \\ -Q_6 & Q_5 & Q_8 & 0 \\ -Q_7 & -Q_8 & Q_5 & 0 \\ Q_8 & -Q_7 & Q_6 & 0 \end{bmatrix}, \tag{59}$$

we can write the regularized momenta, $\mathbf{P}_1$ and $\mathbf{P}_2$, as column vectors with components $(P_1, P_2, P_3, P_4)$ and $(P_5, P_6, P_7, P_8)$, respectively, given by

$$\mathbf{P}_k = \mathbf{A}_k \mathbf{p}_k \qquad (k = 1, 2). \tag{60}$$

Finally, a new time parameter $\tau$ is introduced through the relation

$$dt = R_1 R_2 \; d\tau, \tag{61}$$

having defined $R_1 = |\mathbf{r}_{13}|$, $R_2 = |\mathbf{r}_{23}|$, and $R = |\mathbf{r}_{12}|$. Then the resulting regularized

Hamiltonian reads

$$\Gamma(\mathbf{Q},\mathbf{P}) = \frac{R_2}{8\mu_{13}}\mathbf{P}_1^2 + \frac{R_1}{8\mu_{23}}\mathbf{P}_2^2 + \frac{1}{16m_3}\,\mathbf{P}_1^T\mathbf{A}_1\mathbf{A}_2^T\mathbf{P}_2 - R_2Z_1Z_3 - R_1Z_2Z_3 + R_1R_2\left(\frac{Z_1Z_2}{R} - E\right), \tag{62}$$

where $E$ is the total energy of the system and $\mu_{13}$ and $\mu_{23}$ are the reduced masses of particles 1 and 2 with respect to $m_3$, respectively.

The inter-particle distances $R_1$, $R_2$, and $R$ must be expressed in terms of the regularized coordinates, the relations being

$$R_1 = \sum_{r=1}^{4} Q_r^2, \qquad R_2 = \sum_{r=5}^{8} Q_r^2, \tag{63}$$

and

$$R^2 = R_1^2 + R_2^2 - 2\mathbf{f}_1\cdot\mathbf{f}_2, \tag{64}$$

where the vectors $\mathbf{f}_1$ and $\mathbf{f}_2$ are, expressed in column form,

$$\mathbf{f}_1 = \begin{bmatrix} Q_1^2 - Q_2^2 - Q_3^2 + Q_4^2 \\ 2\,(Q_1Q_2 - Q_3Q_4) \\ 2\,(Q_1Q_3 + Q_2Q_4) \\ 0 \end{bmatrix}, \qquad \mathbf{f}_2 = \begin{bmatrix} Q_5^2 - Q_6^2 - Q_7^2 + Q_8^2 \\ 2(Q_5Q_6 - Q_7Q_8) \\ 2(Q_5Q_7 + Q_6Q_8) \\ 0 \end{bmatrix}. \tag{65}$$

With respect to the Hamiltonian $\Gamma(\mathbf{Q},\mathbf{P};\tau)$, we have the canonical equations of motion

$$\frac{dQ_r}{d\tau} = \frac{\partial\Gamma}{\partial P_r}, \qquad \frac{dP_r}{d\tau} = -\frac{\partial\Gamma}{\partial Q_r} \qquad (r = 1,2,\ldots,8). \tag{66}$$

The explicit form of these equations for the general three-dimensional case is quite cumbersome, although easily obtained with a symbolic-manipulation computer program (such as Maple or Mathematica). It is nonetheless interesting to note that the derivatives $\partial R/\partial Q_i$ can be expressed in a compact form, which is more efficient for numerical purposes. By defining the $8\times 1$ column vector $\mathbf{g}$ as

$$\mathbf{g} = \begin{bmatrix} \mathbf{f}_1 - \mathbf{f}_2 \\ \mathbf{f}_2 - \mathbf{f}_1 \end{bmatrix}, \tag{67}$$

and the $8\times 8$ matrix $\mathbf{A}$

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_1 & \mathbf{0}_4 \\ \mathbf{0}_4 & \mathbf{A}_2 \end{bmatrix}, \tag{68}$$

where $\mathbf{0}_4$ is the null $4\times 4$ matrix, one can write, as can be easily seen [27],

$$\frac{\partial R}{\partial Q_i} = \frac{1}{R}(\mathbf{A}\mathbf{g})_i, \qquad i = 1,2,\ldots,8. \tag{69}$$

### 4.2 Calculation Program

Through the time-scale change, the effect of the regularization is to take very small time steps near the binary collisions ($R_1 \approx 0$ or $R_2 \approx 0$), while keeping a non-divergent Hamiltonian. Our program, developed in C++, uses a standard 4th-order Runge-Kutta adaptive step-size integrator [29] driven by a routine that takes care of coordinate transformations, memory storage, disk swapping of data and Poincaré-section calculations. Poincaré sections are obtained using reverse integration over the trajectory to find the intersection between the orbit and the Poincaré surface instead of interpolation [12].

Initial conditions are defined in laboratory coordinates, integration is performed in the regularized ones, and position output data files are generated in centre-of-mass coordinates for viewing convenience (to eliminate from the plots uniform displacements of the system).

The resulting program, which can be used as a tool for numerical exploration of the general Coulomb three-body problem, produces orbits in reasonable times on a typical desktop computer: usually below one minute for most three-dimensional configurations. The source code is available from the authors upon request.

To conclude our study, we shall finally investigate the numerical feasibility and stability of some configurations that are based on the conclusions drawn in the previous sections. The systems to be studied throughout (with the exception of the $(-)(-)(+)$ and the Poirier configurations) will be the positronium negative ion ($Ps^-$) and the helium atom (He). Atomic units will be used in all discussions.

### 4.3 Collinear Rigid-Rotator Configurations

Let $X$ be the axis on which the three particles lie. If the masses and coordinates (relative to the centre of mass) of our particles are, respectively, $m_i$ and $x_i$ ($i = 1, 2, 3$), and if $\Omega$ is the angular velocity of the system (found using either Eq. (8) or Eq. (13)), then the initial conditions of our problem are

$$\mathbf{r}_i(0) = \big(x_i, 0, 0\big) \tag{70}$$

and

$$\mathbf{p}_i(0) = \big(0, m_i \Omega x_i, 0\big). \tag{71}$$

#### 4.3.1 Orbits and Stability of the Ps$^-$ and the He $(-)(+)(-)$ Configurations

Setting the masses and charges of electron, positron, proton and neutron as $m_{e^-} = m_{e^+} = 1$, $m_p = m_n = 2000$, and $Z_{e^-} = Z_{e^+} = Z_p = 1$, it can be immediately verified that, for both systems, $k = 1$ is the only feasible solution of the 5th-order equation (7). This is of course what should be expected, given the symmetry of these systems. Furthermore, both systems fulfill condition (9). In this fashion, the existence of solutions of the form $(-)(+)(-)$ in $Ps^-$ and He is theoretically guaranteed. The respective values for the rotational angular velocities are $\Omega^2(Ps^-) = \frac{3}{4}$ and $\Omega^2(He) = \frac{7}{4}$.

Table 1 shows the values of initial conditions and the resulting orbit is shown in Fig. 5 a. This configuration is, however, highly unstable. A variation of $10^{-9}$ on one of the initial momenta suffices to cause self-ionization of the system after about two revolutions of the electrons (see Fig. 5 b).

**Table 1.** Initial conditions for the motions of different Coulomb three-body systems in various configurations. The systems are: $Ps^-$ ion, He atom, and the clusters $e^- + F^- + C^{6+}$ and $I^{2-} + 2Kr^{3+}$. The configurations are: symmetric linear rotor (SCR), asymmetric linear rotor (ACR), Langmuir top (LT), Poirier top (PT), fixed-shape solution (FSS), rotating oscillatory solution (ROS) and space-rotating oscillatory solution (SROS)

| System Solution | *i*th particle, $i = 1, 2, 3$ | | | | | |
|---|---|---|---|---|---|---|
| | Coordinates | | | Momenta | | |
| He | −1.0 | 0.0 | 0.0 | 0.0 | −1.32287565 | 0.0 |
| SCR | 1.0 | 0.0 | 0.0 | 0.0 | 1.32287565 | 0.0 |
| | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| $Ps^-$ | −1.0 | 0.0 | 0.0 | 0.0 | 0.86602540 | 0.0 |
| SCR | 1.0 | 0.0 | 0.0 | 0.0 | 0.86602540 | 0.0 |
| | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| $Ps^-$ | −0.28284271 | 0.28284271 | 0.0 | −1.22474487 | −1.22474487 | 0.0 |
| FSS | 0.28284271 | −0.28284271 | 0.0 | 1.22474487 | 1.22474487 | 0.0 |
| | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| $e^- + F^- + C^{6+}$ | −0.28284271 | −0.28284271 | 0.0 | 3.05068571 | −3.05068571 | 0.0 |
| FSS | −0.00505894 | −0.00505894 | 0.0 | 1964.332243 | −1964.332243 | 0.0 |
| | 0.00760020 | 0.00760020 | 0.0 | −1967.382929 | 1967.382929 | 0.0 |
| $e^- + F^- + C^{6+}$ | −1.0 | 0.0 | 0.0 | 0.0 | −2.15716055 | 0.0 |
| ACR | −0.01788607 | 0.0 | 0.0 | 0.0 | −1388.992649 | 0.0 |
| | 0.02687077 | 0.0 | 0.0 | 0.0 | 1391.149810 | 0.0 |
| $Ps^-$ | 0.0 | 0.25887571 | 0.62996052 | −0.44838589 | 0.0 | 0.0 |
| LT | 0.0 | 0.25887571 | −0.62996052 | −0.44838589 | 0.0 | 0.0 |
| | 0.0 | −0.51775143 | 0.0 | 0.89677179 | 0.0 | 0.0 |
| $I^{2-} + 2Kr^{3+}$ | 0.42449697 | 0.0 | 0.70090761 | 0.0 | 547.8170393 | 0.0 |
| PT | 0.20694524 | 0.0 | −0.94509009 | 0.0 | 267.0646390 | 0.0 |
| | −0.41752076 | 0.0 | 0.0 | 0.0 | −814.8816780 | 0.0 |
| $Ps^-$ | −1.0 | 0.0 | 0.0 | 0.70710678 | −0.70710678 | 0.0 |
| ROS | 1.0 | 0.0 | 0.0 | −0.70710678 | 0.70710678 | 0.0 |
| | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| $Ps^-$ | 0.5 | 0.0 | 0.0 | −0.5 | 0.35355339 | 0.5 |
| SROS | −0.5 | 0.0 | 0.0 | 0.5 | −0.35355339 | 0.5 |
| | 0.0 | 0.0 | 0.86602540 | 0.0 | 0.0 | −0.70710678 |

The orbits for the (−)(+)(−) configuration of the helium are analogous to those of $Ps^-$, but it is found that He is more stable than $Ps^-$ for a variation of the same order in the momenta (lifetime of bound He is about twice the lifetime of bound $Ps^-$).

### 4.3.2 The (−)(−)(+) Configuration

As already stated before, it is impossible for $Ps^-$ or He to conform to a (−)(−)(+) configuration. We must look instead for systems having either $m_1 \neq m_2$ or $Z_1 \neq Z_2$ (or, in general, systems fulfilling condition (12)). One particular such system is the one given by $(m_1, m_2, m_3) = (1, 36000, 24000)$ and $(Z_1, Z_2, Z_3) = (1, 1, 6)$, which can be thought as formed by an electron, a $_{18}F^-$ ion and a nucleus of $_{12}C^{6+}$. This system has also the desired characteristic of yielding two positive roots to the 5th-order equation (11), namely $\{k_1, k_2\} = \{0.04557195, 1.449132205\}$, and only the first of these roots fulfills condition (14), producing a value of $\Omega_1^2 = 4.653341$. From this and the fixed inter-particle ratios, the initial conditions can be deduced, giving the

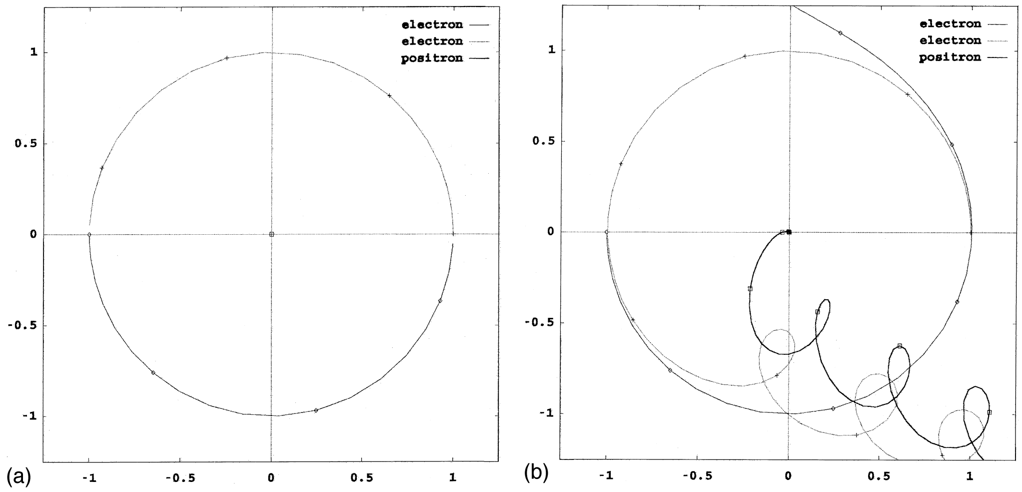


**Fig. 5.** **a**: Collinear symmetrical configuration of the positronium negative ion $Ps^-$. The positron is fixed at the origin of coordinates. **b**: Small variation on the (−)(+)(−) configuration for the $Ps^-$

results presented in Table 1. The trajectories followed by the particles can be seen in Fig. 4 a.

This configuration is surprisingly stable: The system remains bound for variations (transversal and radial) of the order of unity on the momentum of particle 1 (the electron), and particles 2 and 3 admit variations as great as $10^3$ in their momenta. On the other hand, variations of the order of unity on the $x_1$ coordinate, and of the order of $10^{-2}$ on the $x_2$ and $x_3$ coordinates, cause the system to self-ionize. In Fig. 4 b, a variation of $10^2$ on the radial momentum of particle 2 is shown.

### *4.4 In-Plane Rotating-Oscillatory Configurations*

The configurations to be numerically explored in this section are those in which the distances between particles "oscillate" (or, in general, have an initial inwards momentum) on a given initial direction in the plane of the particles, while rotating about a fixed ($Z$) axis. Fixed-shape solutions conform to a particular subset of such configurations. In this manner, we shall deal with the collinear (−)(+)(−) and (−)(−)(+) configurations. Afterwards, the three-dimensional (in-plane) rotating-oscillatory configurations will be examined, both in the cases in which the shape of the triangle (assumed to be equilateral at $t = 0$) is preserved as time evolves, and in the case in which it is not. The system to be studied in detail is $Ps^-$, but some comments on He will be made too (especially regarding its stability compared to that of the $Ps^-$).

#### 4.4.1 Fixed-Shape Configurations

A complete family of solutions derived from each of the two types of linear rigid configurations was obtained in Sect. 3. Different members of the families are identified by the parameters of the Kepler motion in Eq. (53); these arbitrary parameters are the amplitude $a$, eccentricity $e$ and perihelion angle $\delta$, and they identify members of

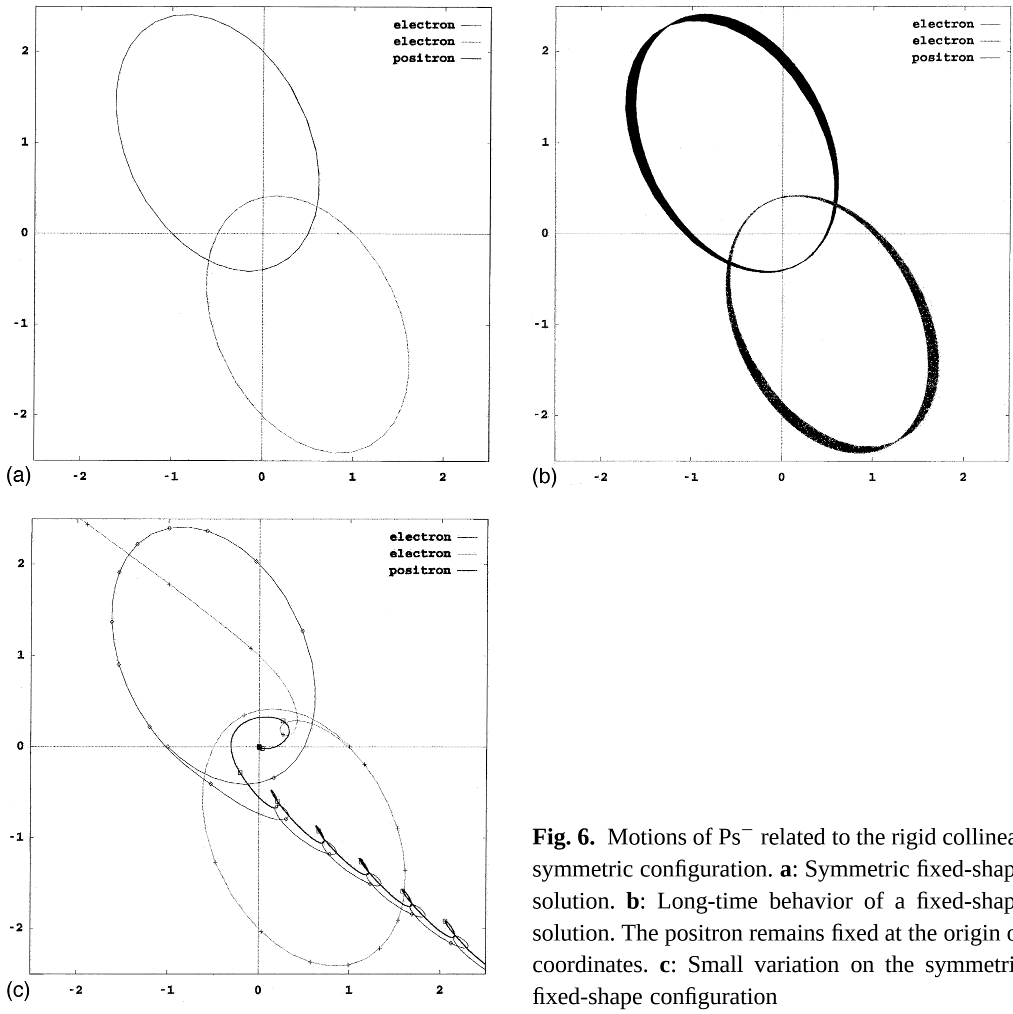


**Fig. 6.** Motions of $Ps^-$ related to the rigid collinear symmetric configuration. **a**: Symmetric fixed-shape solution. **b**: Long-time behavior of a fixed-shape solution. The positron remains fixed at the origin of coordinates. **c**: Small variation on the symmetric fixed-shape configuration

complete families of solutions. If the motion is observed in a frame rotating with angular velocity $\Omega$, the rigid solutions appear as fixed points and the fixed-shape solutions as oscillations around those points.

Fig. 6 a shows one fixed-shape solution derived from the collinear $(-)(+)(-)$ configuration of $Ps^-$ and Fig. 4 d shows one fixed-shape solution derived from the collinear asymmetric configuration of $e^- + {}_{18}F^- + {}_{12}C^{6+}$.

### 4.4.2 Three-Dimensional (In-Plane) Rotating Oscillatory Configurations

Let $X$ be the axis on which the two electrons lie at $t = 0$ (located symmetrically on both sides of the origin), and $Z$ the axis on which the positron is located at this same time. If $\Omega$ and $\omega$ are, respectively, the initial rotating angular velocity (about $Z$) and angular frequency of the oscillations, and if the initial direction of oscillation $\theta$ for each electron (relative to the $X$ axis) is the $Z$-mirror of the direction for the other electron (while $-Z$ is the initial direction of oscillation for the positron), then the more general conditions for the initial equilateral-triangle configuration (side = $r$) are

$$\mathbf{r}_1(0) = (-r/2, 0, 0),$$
$$\mathbf{r}_2(0) = (r/2, 0, 0),$$
$$\mathbf{r}_3(0) = \left(0, 0, r\sqrt{3}/2\right) \tag{72}$$

and

$$\mathbf{p}_1(0) = \left(m_1\xi_o\omega\cos\theta, m_1\Omega x_1, m_1\xi_o\omega\sin\theta\right),$$
$$\mathbf{p}_2(0) = \left(-m_2\xi_o\omega\cos\theta, m_2\Omega x_2, m_2\xi_o\omega\sin\theta\right),$$
$$\mathbf{p}_3(0) = \left(0, 0, -m_3\xi_o\omega\right), \tag{73}$$

where $\xi_o$ is some parameter representing the amplitude of the oscillations. In this fashion, using $m_1 = m_2 = m_3 = 1$, $Z_1 = Z_2 = Z_3 = 1$, $r_{ij}(0) = 1$ $(i, j = 1, 2, 3)$, and making, for example, $\Omega^2 = \omega^2 = \frac{1}{2}$ and $\xi_o = 1$, our initial conditions are completely determined for a given value of $\theta$.

If we put $r = 1$ and $\theta = 30^\circ$ in Eqs. (72) and (73), the resulting orbits are those of Fig. 7 a. It is interesting to observe the $XY$, $XZ$, and $YZ$ projections of these orbits. The enlightening $XY$ projection is shown in Fig. 7 b.

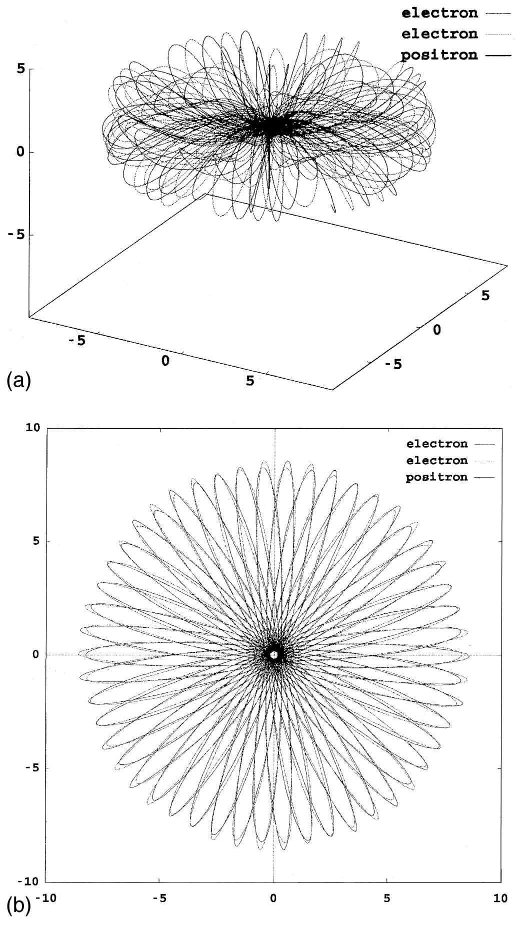


**Fig. 7.** Three-dimensional rotating oscillatory (−)(+)(−) configuration of the $Ps^-$. The positron follows a rectilinear trajectory. **a**: Rotating oscillatory equilateral triangle for the $Ps^-$. **b**: Projection $XY$

Another noteworthy configuration (also in the form of a triangle) is the slowly-rotating and quasi-rigid one, in which $\Omega^2 = 0.1$, $\omega^2 = 0.9$, and $\xi_o = 0.01$. All these configurations are very unstable. For helium, things are not better. The system undergoes self-ionization after two revolutions when subjected to a variation of the order of $10^{-9}$ on one of its momenta.

If now, instead of choosing $\theta = 30^\circ$, we put, for example, $\theta = 45^\circ$ in Eqs. (72) and (73), the triangle will leave its original equilateral configuration when "time is turned on." However, the numerical results show that bound orbits can also be found with stabilities of the same order as those corresponding to the configuration obtained setting $\theta = 30^\circ$.

### 4.5 Rigid Top Configurations

Formulas derived from Eq. (38) for Poirier top must be numerically solved in order to obtain the initial conditions given in Table 1 (see Fig. 3 b).

General initial conditions for Langmuir top solution can be expressed analytically by

$$\begin{aligned}
\mathbf{r}_1(0) &= \big(m_3h/m, h\Delta, 0\big),\\
\mathbf{r}_2(0) &= \big(m_3h/m, -h\Delta, 0\big),\\
\mathbf{r}_3(0) &= \big(-2m_1h/m, 0, 0\big),\\
\mathbf{p}_1(0) &= \big(0, 0, -a\omega m_1\big),\\
\mathbf{p}_2(0) &= \big(0, 0, -a\omega m_1\big),\\
\mathbf{p}_3(0) &= \big(0, 0, 2a\omega m_1\big),
\end{aligned} \tag{74}$$

where $m_1 = m_2$, $Z_1 = Z_2$, $\omega$ is the rotation frequency, $h$ is the distance from particle 3 to the centre of mass of the other two particles, $a = m_3h/m$, and $\Delta = [-1 + (4Z_3/Z_1)^{2/3}]^{-1/2}$. This means that $Z_1 \leq 4Z_3$. $h$ can also be expressed as a function of angular momentum in the form

$$h = \frac{2m}{m_1m_3^2}\,\frac{\Delta^3}{Z_1^2}L^2. \tag{75}$$

## 5 Conclusions and Open Questions

In this work, some analytic and general studies of the Coulomb three-body problem were performed. In particular, regarding the existence of rigid-rotator and fixed-shape solutions, necessary and/or sufficient conditions (involving the dynamical and geometrical parameters of the system) were deduced. Besides, some expressions from which physically relevant quantities (e.g., inter-particle distance ratios, rotational angular velocities) of these configurations can be inferred were also found.

The general results of Sects. 2 and 3 are, up to the authors' knowledge, new. Even though the impossibility of the existence of a plane rigid rotating solution for the Coulomb three-body problem had been mentioned as an intuitive physical fact (see ref. [9]), its proof has only been given in the present work.

Through the numerical exploration of some particular systems, Sect. 4 shows the existence of the configurations predicted by the theory developed in Sects. 2 through 3, as well as some in-plane oscillating-rotating three-dimensional solutions. This last kind of solutions lacks a general theoretical analysis, while the methods of Sect. 3 are a first approach to their study. Sect. 4 also shows that most of the orbits involving a high degree of symmetry in the initial conditions are very unstable, whereas non-symmetric configurations [as the $(-)(-)(+)$] are significantly more stable.

This work leaves many open questions. Some of them are:

- In order to perform an analytic stability analysis of the general collinear configurations, it would be necessary to know the solution to the general 5th-order equations (7) and (11). Even though this task is not feasible (as demonstrated by the mathematician Abel), perhaps conditions (9), (12), and (14), which establish some mathematical constraints on these 5th-order equations so that they have physically meaningful roots, could help to draw more particular conclusions related to these relevant roots.
- The system $e^- + {}_{18}F^- + {}_{12}C^{6+}$ studied numerically in Sect. 4, is hardly obtainable in real physical situations. It would therefore be desirable to study other systems with a more realistic experimental feasibility.
- The static configuration and the corresponding uniform-motion solution, which conforms to real systems like $Be^{4+} + e^- + Be^{4+}$, could be explored by using quantum mechanics in order to determine its experimental relevance. This configuration could also be relevant for the trapping of a classical electron between two heavy centres in collisions of the $Be^{3+}$ and $Be^{4+}$ ions.
- A special case involving a triple collision was found in this work. It shows the possible relevance of studies on the regularization of general triple collisions.

*Acknowledgments.* Support from the Centro de Investigaciones en Ciencias Exactas y Naturales of the Universidad de Antioquia, CIEN, the International Centre for Theoretical Physics, ICTP, and Colciencias under contract No. Co: 1115-05-012-92, is gratefully acknowledged.

## References

1. Aarseth, S. J., Zare, K.: Celest. Mech. **10**, 185 (1974)
2. Armour, E. A. G., Brown, W. B.: Acc. Chem. Res. **26**, 168 (1993)
3. Barnett, R. A.: College Algebra with Trigonometry. New York: McGraw-Hill 1984
4. Blitzer, L.: Cel. Mech. **42**, 215 (1988)
5. Botero, J.: Phys. Rev. **A35**, 36 (1987)
6. Brandsen, B. H., Joachain, C. J.: Physics of Atoms and Molecules. Harlow, Essex: Longman Scientific & Technical 1983
7. Broucke, R., Anderson, J. D., Blitzer, L., Davoust, E., Lass, H.: Celest. Mech. **24**, 63 (1981)
8. Dimitrijević, M. S., Grujić, P. V.: Z. Naturforsch. **39a**, 930 (1984)
9. Grujić, P. V.: Bull. Astron. Belgrade **147**, 15 (1993)
10. Grujić, P. V., Simonović, N. S.: Phys. Rev. **A50**, 4836 (1994)
11. Heggie, D. C.: Mon. Not. R. Astron. Soc. **173**, 729 (1975)
12. Hénon, M.: Physica **D5**, 412 (1982)
13. Hietarinta, J., Mikkola, S.: CHAOS **3**, 183 (1993)
14. Hut, P., Bahcall, J. N.: Astrophys. J. **268**, 319 (1983)
15. Jensen, R. V., Leopold, J. G., Richards, D.: J. Phys. **B21**, L527 (1988)
16. Klar, H.: J. Phys. **B14**, 3255 (1981)
17. Klar, H.: Z. Phys. **D3**, 353 (1986); J. Opt. Soc. Am. **B4**, 788 (1987)
18. Kustaanheimo, P., Steifel, E.: J. Reine Angew. Math. **218**, 204 (1965)
19. Mahecha, J.: J. Phys. **B37**, 1925 (1994)

20. Marchal, C.: The Three-Body Problem (Studies in Astronautics, Vol. 4). Amsterdam: Elsevier 1990
21. Martin, A., Richard, J.-M., Wu, T. T.: Phys. Rev. **A43**, 3697 (1992)
22. Martin, A., Richard, J.-M., Wu, T. T.: Phys. Rev. **A52**, 2557 (1995)
23. Martínez, J. C.: Am. J. Phys. **63**, 2 (1995)
24. Pars, L. A.: A Treatise on Analytical Dynamics. London: Heinemann 1965
25. Percival, I. C., Richards, D.: J. Phys. **B3**, 1035 (1970)
26. Percival, I. C.: Proc. R. Soc. Lond. **A353**, 289 (1977)
27. Pérez, F., Mahecha, J.: Rev. Méx. Fís. **42**, 1552 (1996)
28. Poirier, M.: Phys. Rev. **A40**, 3498 (1989)
29. Press, W. H., Teukolsky, S. A., Vetterling, W. T., Flannery, B. P.: Numerical Recipes in C. Cambridge: Cambridge University Press 1988
30. Richter, K., Tanner, G., Wintgen, D.: Phys. Rev. **A48**, 4182 (1993)
31. Thatcher, A.: Eur. J. Phys. **3**, 202 (1982)
32. Yamamoto, T., Kaneko, K.: Phys. Rev. Lett. **70**, 1928 (1993)

Received February 27, 1996; revised September 2, 1996; accepted for publication October 22, 1996