Classical Coulomb three-body problem in collinear eZe configuration

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Abstract. Classical dynamics of two-electron atom and ions H−, He, Li+, Be2+, ... in collinear eZe configuration is investigated. We consider the case that the masses of all particles are finite. It is revealed that the mass ratio ξ between nucleus and electron plays an important role for dynamical behaviour of these systems. With the aid of analytical tool and numerical computation, it is shown that thanks to large mass ratio ξ, classical dynamics of these systems is fully chaotic, probably hyperbolic. Experimental manifestation of this finding is also proposed.

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1. Introduction

Three-body problem in celestial mechanics is one of pioneer studies on chaotic phenomena and, at the same time, one of the oldest and the most famous problems in physics. First systematic work has been given by Poincaré, for which he won the prize established by King Oscar II of Sweden and Norway (Poincaré, 1899). Main result of his work is that the motion of three particles is very complicated (i.e., what we now call "chaos") and then it is generally hard to solve it practically. After Poincaré, many mathematicians and physicists contributed to this problem (See, for instance, the book (Siegel and Moser, 1971) as mathematical literature.). In addition, innovation of computers assisted physicists to investigate this problem. However, our understanding of three-body problem is far from complete. The investigation is still going on.

Three-body problem also exists in Coulomb systems. The most popular Coulomb three-body system is helium atom which consists of one nucleus and two electrons. In early stage of making quantum mechanics, many physicists did not know what to do with the spectrum of helium atom, in spite of success of explaining of the spectrum of hydrogen atom. For hydrogen atom, stable periodic orbits correspond to eigen energies of it. This correspondence is now called the Bohr-Sommerfeld (BS) quantization. However, they could not explain the spectrum of helium atom by the BS-quantization scheme. Einstein extended the BS-quantization to higher-dimensional classically integrable case (now we call it the Einstein-Brioullin-Keller (EBK) quantization.) and pointed out indirectly this problem of helium atom (i.e., not integrable case) referring to the work by Poincaré (Einstein, 1917). About fifty years later, Gutzwiller succeeded to derive an approximate quantization condition for hyperbolic cases. His formula expresses the density of states in terms of unstable periodic orbits, which is now called the Gutzwiller trace formula (Gutzwiller, 1971, 1990). In early 90's, several physicists applied the Gutzwiller trace formula to hydrogen negative ion (Gaspard and Rice, 1993) and helium atom (Ezra et al., 1991) in collinear configuration, i.e., restricted Coulomb three-body problem. Series of these studies showed that these atom and ions in collinear eZe configuration are fully chaotic, probably hyperbolic and the Gutzwiller trace formula yields nice approximate values for series of eigen energies with angular momentum $L = 0$ numerically (See also the review (Tanner, Richter and Rost, 2000).). Here “e” and “Z” represent electron and nucleus, respectively. Thus “eZe” stands for the order of particles on a line. Their work has left a question why hydrogen negative ion and helium atom in collinear eZe configuration are fully chaotic. We used the term “fully chaotic” in the meaning that almost all periodic orbits are hyperbolic. Thus, we used the term “fully chaotic” for the system which is almost chaotic, but possesses small tiny island. In addition, we shall use the term “hyperbolic” in the meaning that all periodic orbits are hyperbolic.

It was numerically shown that if the mass of nucleus is infinite for eZe collinear configuration, the symbolic description of it is complete for the negative energy $E < 0$ and $Z \geq 1$ (Bai, Gu and Yuan, 1998). This result suggested that for the infinite nucleus
mass, the dynamics is hyperbolic.

In this paper, we consider the case that all masses are finite and numerically confirm that the dynamics of two-electron atom and ions in collinear eZe configuration, i.e., H+, He, Li+, Be2+, ... is hyperbolic. Parameters of these systems are the mass ratio \( \xi = m_n/m_e \) and the charge \( Z \) of nucleus, where \( m_n(m_e) \) are the mass of nucleus(electron), respectively. We employ numerical computation for these systems with the aid of analytical tool(the triple collision manifold(TCM)) (McGehee, 1974) and symbolic dynamics(Tanikawa and Mikkola, 2000) from celestial mechanics. The TCM is a manifold which is a set of the initial or final conditions of the triple collision orbit, i.e., thus just the triple collision points. The flow on the TCM does not have physical reality, because the TCM corresponds just triple collisions. However, the flow on the TCM affects the flow near the TCM because of the continuous property of the solution for the equations of motion. Thus, we can study the behaviour near the triple collision from the flow on the TCM. It is shown that the mass ratio \( \xi \) plays an important role for dynamical behaviour of these systems. In precise, sufficiently large mass ratio \( \xi \) makes the system be fully chaotic. Therefore it is revealed that all of these systems are fully chaotic, probably hyperbolic, since the mass ratio is sufficiently large, e.g., \( m_p/m_e \approx 1840 \), where \( m_p \) is the mass of proton.

We confirm this result as follows: First, we elucidate the \( \xi \)-dependence of the local structure near the triple collision by examining the flow on the TCM. In particular, we investigate the stable(or unstable) manifold of two critical points on the TCM. By this analysis, we show the change of the triple collision orbit when \( \xi \) is increased. Let us denote the winding number of the stable(or unstable) manifold (on the TCM) of the critical point around the body of the TCM by \( \mathcal{N} \). Later we shall define the body of the TCM precisely. It is shown that when \( \xi \to 0 \), \( \mathcal{N} \) becomes infinite and, in the opposite limit, when \( \xi \) is increased, \( \mathcal{N} \) is decreased and saturated to certain values. Second, we examine the morphology of the Poincaré surface of section using the associated symbolic dynamics. The symbolic dynamics is naturally introduced by labeling the double collision between the particles 1 and 2(2 and 3) by symbol 1(2), respectively. The position of the triple collision orbits on the Poincaré surface of section is specified. When \( (Z, \xi) = (1, 1) \), there is a torus on the Poincaré surface of section, whose corresponding sequence of symbols is \( \ldots 12121212 \ldots \). The triple collision orbits forms curves on the Poincaré surface of section. We call these curves the triple collision curves \( \mathcal{C}_{TC} \). In this case, \( \mathcal{C}_{TC} \) crosses its reversed pair \( \mathcal{C}_{TC}^r \) transversely except near the torus. \( \mathcal{C}_{TC}^r \) is mapped to \( \mathcal{C}_{TC} \) by the symmetry operation due to the reverse operation. For helium \( (Z, \xi) = (1, 4m_p/m_e) \), there is no torus. \( \mathcal{C}_{TC} \) crosses its pair \( \mathcal{C}_{TC}^r \) transversely everywhere. From numerical calculation, \( \mathcal{C}_{TC}(\mathcal{C}_{TC}^r) \) is parallel to the stable manifolds(unstable manifolds) in the Poincaré section for the Poincaré map, respectively. Therefore, this fact is an strong evidence that the stable and unstable manifolds transversely cross each other for the case of helium in collinear eZe configuration. In addition, we show the relationship between the structure of the stable and unstable manifolds of two critical points on the TCM and \( \mathcal{C}_{TC} \) and \( \mathcal{C}_{TC}^r \) on the Poincaré section. At this time, it is turned
out that the change of the triple collision orbit on the TCM w.r.t ξ is related to the collapse of the torus whose corresponding symbol sequence is . . . 121212 . . . . The above facts strongly suggest that two-electron atom and ions in collinear eZe configuration is fully chaotic, probably hyperbolic.

The organization of this paper is as follows. In §2, the Hamiltonian of the systems considered in this paper is introduced. Due to the attractive interaction between neighbouring particles, double collisions surely occur. Therefore, an regularization is required before numerical computation. We choose an algorithmic regularization not analytical regularization such as Kustaanheimo-Stiefel transformation or Levi-Civita transformation. In §3 the TCM is introduced. The ξ-dependence of the flow on the TCM is numerically investigated. In particular, the change of the triple collision orbit w.r.t. ξ is shown. In §4, method of symbolic dynamics is applied to the systems for the case Z = 1 and ξ = 1 and the case of helium. In the former case, there is a torus whose symbol sequence is . . . 121212 . . . . We examine the topological character of this system in detail. On the other hand, in the case of helium, there is no torus whose corresponding symbol sequence is . . . 121212 . . . . In fact, the corresponding orbit for the symbol sequence . . . 121212 . . . is an isolated unstable periodic orbit. With the result of §3, what this observation means is considered. In §5, the results of this paper is summarized.

2. Hamiltonian and regularization

We consider three particles 1, 2 and 3 whose masses are $m_1 = m_e$, $m_2 = m_n = \xi m_e$, and $m_3 = m_e$ and whose charges are $-e$, Ze, and $-e$, respectively. The mass ratio $\xi$ is given by $\xi = m_n/m_e$. The Hamiltonian for this system is

$$H = \sum_{i=1}^{3} \frac{p_i^2}{2m_i} - \frac{Ze^2}{|q_1 - q_2|} - \frac{Ze^2}{|q_2 - q_3|} + \frac{e^2}{|q_1 - q_3|}. \quad (1)$$

Now we employ the famous scaling for Coulomb systems.

$$q_i = \alpha q'_i, \quad p_i = \beta p'_i, \quad E = \gamma E'$$

with

$$\alpha = \frac{Z}{m_e e^2 |E|}, \quad \beta = |E|^{1/2} m_e e^2, \quad \gamma = m_e e^4. \quad (3)$$

$E$ is the value of the Hamiltonian $H$. After this scaling, we get the following Hamiltonian.

$$\mathcal{H} = \frac{p_1'^2}{2} + \frac{p_2'^2}{2\xi} + \frac{p_3'^2}{2} - \frac{1}{|q_1' - q_2'|} - \frac{1}{|q_2' - q_3'|} + \frac{1}{Z|q_1' - q_3'|} = E' = -1. \quad (4)$$

For simplicity, we set $E' = -1$. Now the particles are arranged in the order $q'_1 \leq q'_2 \leq q'_3$. If we set $(Z, \xi) = (-1, 1)$, the system is equivalent to the system which was investigated in gravitational three-body problem (Tanikawa and Mikkola, 2000). We set the total momentum to be zero and change the variables $q'_i$’s to

$$Q_1 = q'_2 - q'_1, \quad Q_2 = q'_2, \quad Q_3 = q'_3 - q'_2. \quad (5)$$
with new momenta
\[ P_1 = -p'_1, \quad P_2 = p'_1 + p'_2 - p'_3, \quad P_3 = p'_3. \] (6)
This canonical transformation is generated by the following generating function \( W \).
\[ W = P_1(q'_2 - q'_1) + P_2q'_2 + P_3(q'_3 - q'_2). \] (7)
The final form of the Hamiltonian \( \mathcal{H} \) is
\[ \mathcal{H} = \frac{P_1^2}{2\mu} + \frac{P_2^2}{2\mu} - \frac{P_1P_2}{\xi} - \frac{1}{Q_1} - \frac{1}{Q_2} + \frac{1}{Z(Q_1 + Q_2)} = -1, \] (8)
with \( \mu = \xi/(\xi + 1) \). After the canonical transformation, we replaced \((P_3, Q_3)\) by \((P_2, Q_2)\) for convenience. The parameters of this Hamiltonian is the charge \( Z \) and the mass ratio \( \xi \).

The potential in Eq.(8) has singularities associated to double collisions of particles. Thus appropriate regularization is needed. To regularize them, in celestial mechanics a transformation such as Kustaanheimo-Stiefel transformation or Levi-Civita transformation is usually employed. However, an algorithmic regularization (Mikkola and Tanikawa, 1999) is used here. A merit of this choice is that for accurate numerical integration of equations of motion, the symplectic integrator method can be used (Yoshida, 1990). For usual analytical regularization, the symplectic integrator method can not be applied, since there are coupling terms of position and momentum in the Hamiltonian, i.e., the Hamiltonian after the transformation mentioned above is not a summation of the form \( \mathcal{H} = T(P) + V(Q) \). We will use the sixth order symplectic integrator method in §4. After regularization, double collision is extended to just elastic collision and triple collision is not regularized in general. The interaction between outer particles and middle one is attractive, while the interaction between outer particles is repulsive. Thus neighbouring particles are always attracted and collide each other. Hence the trajectory of three particles is, in general, a sequence of collisions. Among collisions, triple collisions exist as very rare events. In fact, the measure of set of triple collisions would be zero. However, the triple collisions form the bone structure of dynamics of our systems which we will see in §3 and §4.

Here the symbolic coding of the orbit which will be extensively used in §4 is introduced briefly. Let us denote the whole set of orbits in our systems by \( \mathcal{O} \). The set \( \mathcal{O} \) is a union of \( \mathcal{O}_{DC} \) and \( \mathcal{O}_{TC} \), where \( \mathcal{O}_{DC} \) is the set of orbits which only consist of double collisions and \( \mathcal{O}_{TC} \) is the set of orbits which include triple collisions.
\[ \mathcal{O} = \mathcal{O}_{DC} \cup \mathcal{O}_{TC}. \] (9)
For an orbit of \( \mathcal{O}_{DC} \), it is natural that the double collision with the particle 1 and 2(2 and 3) is labeled by symbol 1(2), respectively. Therefore, the symbol set for \( \mathcal{O}_{DC} \) is \( A_0 = \{1, 2\} \). Let us express an given orbit of \( \mathcal{O}_{DC} \) as a sequence of symbols as follows:
\[ n = \ldots n_{-2}n_{-1} \cdot n_0n_1n_2 \ldots, \] (10)
where \( n_i \in A_0, i \in \mathbb{Z} \). In order to describe an orbit of \( \mathcal{O}_{TC} \) as a symbol sequence, we need another symbol, i.e., 0. We set \( A = \{0, 1, 2\} \). The triple collision orbit is started
and/or ended by the triple collision. Let us label the triple collision by symbol 0. The orbit which experiences the triple collision cannot be continued. Thus we regard as 0 continuing endlessly after the first 0 in the future and before the last 0 in the past, if 0 appears in the sequence. For example, a triple collision orbit is represented as

\[ n = \ldots 000n_{-l}n_{-(l-1)} \ldots n_{-1} \cdot n_0n_1n_2 \ldots, \quad (11) \]
or

\[ n = \ldots n_{-3}n_{-2}n_{-1} \cdot n_0n_1 \ldots n_m000 \ldots, \quad (12) \]
or

\[ n = \ldots 000n_{-l}n_{-(l-1)} \ldots n_{-1} \cdot n_0n_1 \ldots n_m000 \ldots, \quad (13) \]

where \( n_i \in A_0 \). The shift operator \( \sigma \) on \( A^Z \) is defined by

\[ \sigma(\ldots n_{-2}n_{-1} \cdot n_0n_1n_2 \ldots) = \ldots n_{-2}n_{-1}n_0 \cdot n_1n_2 \ldots. \quad (14) \]

We sometimes call finite symbol sequence the word. For instance, 12 and 1211 are words.

3. Triple collision manifold

The triple collisions are, in general, essential singularities and thus are not regularized. They are rare events. Therefore, it is hard to visualize the triple collisions. In order to investigate the structure near the triple collision, technical method is required. For celestial problem, McGehee has developed such method (McGehee, 1974). He has derived the equations of motion for the flow just on the triple collision. Its derivation is successive application of tricky transformations to the equations of motion Eq.(4) and the energy conservation relation \( H = T(p) - U(q) = E \). A manifold on which the orbit experiences just the triple collision is obtained by setting the moment of inertia to be zero (i.e., just triple collision) in the final energy conservation relation. This substitution is meaningful owing to tricky transformations (i.e., scalings and time-transformations). This manifold is called the triple collision manifold (TCM). Thanks to similarity between celestial problem and Coulomb problem, this method can be also applied to our Coulomb problem. Since the transformations are tricky and complicated, in order to be self-contained, we show the derivation of it rapidly in the Appendix. For the detail of the derivation, the readers are recommended to consult with the article (McGehee, 1974). Starting from the energy conservation Eq.(4) and the equations of motion for Eq.(4), after lengthy calculation (i.e., six times of changes of variables), we obtain the energy conservation relation with \( r = 0, \) i.e., the moment of inertia \( r^2 = q_1^2 + \xi q_2^2 + q_3^2 \) is zero (just the triple collision) or with alternately the total energy \( E = 0 \) : \[ w^2 + s^2 - 1 + (1 - s^2)^2W(s)^{-1}v^2 = 0. \quad (15) \]

Equation (15) defines a surface in \((s, v, w)\)-coordinates, i.e., the TCM. The TCM is topologically equivalent to a sphere with four holes. Schematic picture for the TCM \( \frac{r}{E} \) and \( E \) appears as a term \( rE \) in the energy relation and equations of motion (See the Appendix.). Therefore, the TCM and the flow on the TCM are the same for either \( r = 0 \) and \( E = 0 \).
is depicted in Fig. 1. For the definition of $s, v, w, W(s)$, see the Appendix. We only explain what $s$ represents. $s$ represents the configuration of three particles. $s$ is valued in $[-1, 1]$. $s = -1 (s = 1)$ corresponds to the double collision between the particles 1 and 2 (2 and 3), respectively. The flow on the TCM is determined by the following equations of motion

$$
\frac{dv}{d\tau} = \frac{\lambda}{2} W(s)^{1/2} \left[ 1 - \frac{1 - s^2}{W(s)} v^2 \right],
$$

$$
\frac{ds}{d\tau} = w,
$$

$$
\frac{dw}{d\tau} = - s + \frac{2s(1 - s^2)}{W(s)} v^2 + \frac{1}{2} \frac{W'(s)}{W(s)} (1 - s^2 - w^2) - \frac{\lambda}{2} \frac{1 - s^2}{W(s)^{1/2}} vw.
$$

(16)

For the definitions of $\lambda, s, v, w,$ and $\tau$, see the Appendix. There are two critical points $c = (0, -v_c, 0)$ and $d = (0, v_c, 0)$, two infinite arms ($a$ and $b$), and two infinite legs ($e$ and $f$), where $v_c = W(0)^{1/2}$. Most of orbits on the TCM comes from infinity of one of two legs winding around it and goes out to infinity of one of two arms winding around it.

There is an important property for the orbits with $r \neq 0$ (i.e., for total flow).

**Property 3.1:** For $\mathcal{H} = E < 0$, the orbits runs inside of the TCM, i.e., $w^2 + s^2 + (1 - s^2)^2 W(s)^{-1} v^2 \leq 1$. On the other hand, for $\mathcal{H} = E > 0$, the orbits runs outside of the TCM, i.e., $w^2 + s^2 + (1 - s^2)^2 W(s)^{-1} v^2 \geq 1$.

Here after we consider the case of $\mathcal{H} = E < 0$.

If the orbit crosses $s = -1 (s = 1)$, the corresponding trajectory in the configuration space experiences the double collision between the particles 1 and 2 (2 and 3) with the symbol 1 (2), respectively. After some collisions they are going out to infinity by changing its binary or not. There also exist the triple collision orbits. By definition, the triple collision orbits are the orbits which start/end at the TCM (i.e., $r = 0$). This means that the triple collision orbit can not be regularized, that is, the triple collision orbits can not continue after/before the triple collisions. As shown by McGehee (McGehee, 1974), the triple collision orbits form one parameter family. This fact is understood from the stability analysis of the critical point $c$ and $d$. The critical points $c$ and $d$ are the fixed points of the flow Eq. (16). At the same time, they are the fixed points of the total flow Eq. (16), which is not restricted to $r = 0$. The stability analysis of the fixed points $c$ and $d$ shows that $\dim(W^s(c)) = 2$, $\dim(W^u(c)) = 1$ and $\dim(W^s(d)) = 1, \dim(W^u(d)) = 2$, where $W^s(x)$ and $W^u(x)$ are the stable and unstable manifolds of $x$, respectively. In Fig 2 the schematic picture of $W^s(c), W^u(c), W^s(d),$ and $W^u(d)$ is depicted. One branch of $W^s(c)$ (we call it $W^{s*}(c)$) comes into $c$ on the TCM from the outside of the TCM (i.e., $r \neq 0$) along the $v$-axis. Similarly, one branch of $W^u(d)$ (we call it $W^{u*}(d)$) goes out $d$ on the TCM to the outside of the TCM (i.e., $r \neq 0$) along $v$-axis. The other branch of $W^s(c)$ and $W^u(c)$ (we call them $W_{TCM}(c)$) runs on the TCM and winds around the TCM. Similarly, the other branch of $W^u(d)$ and $W^s(d)$ (we call them $W_{TCM}(d)$) runs on the TCM and winds around the TCM. In the outside of the TCM (i.e., $r \neq 0$) near the critical point $c$ and $d$, there exists one parameter family of the orbits which approach to $W_{TCM}(c)$ as $\tau \to \infty$. Similarly, there exists one parameter family of the
orbits which escape from $\mathcal{W}_{TCM}(d)$ as $\tau \to \infty$. Therefore, $\mathcal{W}_{TCM}(c)$ and $\mathcal{W}_{TCM}(d)$ determine the behaviour of the triple collision orbits. Unfortunately, this discussion here is limited to the neighbourhood of the critical points $c$ and $d$(i.e., local property). In the next section, we investigate $\mathcal{W}_{TCM}(c)$ and $\mathcal{W}_{TCM}(d)$ numerically to show the global topological property of the triple collision orbits. For later use, we call the part of the TCM between two critical points $c$ and $d$ the body of the TCM, in precise, \{(s, v, w); -v_c \leq v \leq v_c, (s, v, w) \text{ on the TCM}\}.

Our interest in this section is focused on the $\xi$-dependence of the flow on the TCM. In the celestial problem in collinear configuration considered in the section 10 of the article(McGehee, 1974), it is shown that for the case of $m_1 = m_3 = m$ and $m_2 = \epsilon m$, when $\epsilon \to 0$, the orbits on the TCM wind around the TCM infinitely. Thanks to the similarity between celestial problem and Coulomb problem, for our Coulomb systems, the same argument is easily shown following the discussion of the article(McGehee, 1974).

**Property 3.2:** When $\xi \to 0$, the orbits on the TCM wind around the body of the TCM infinitely often.

This is due to the fact that $\frac{dv}{d\tau} \to 0$ as $\xi \to 0$. The proof is the same as the Proposition 10.1 of the article(McGehee, 1974).

In order to show the $\xi$-dependence of the flow on the TCM for large $\xi$, we numerically calculate $\mathcal{W}_{TCM}(c)$ and $\mathcal{W}_{TCM}(d)$. For this numerical integration of Eq.\,(10), we used the fourth order Runge-Kutta method. Figure 3 depicts $\mathcal{W}_{TCM}(c)$ and $\mathcal{W}_{TCM}(d)$ for $(Z, \xi) = (1, 1)$. Figures 4(a) and (b) depict one branch(the unstable manifold) of $\mathcal{W}_{TCM}(c)$ for the cases $(Z, \xi) = (1, 0.1)$ and $(1, 6)$, respectively. The change of $\mathcal{W}_{TCM}(c)$ w.r.t. $\xi$ is clearly seen in Fig 4. When $\xi$ is increased, the winding number $N$ of $\mathcal{W}_{TCM}(c)$ or $\mathcal{W}_{TCM}(d)$ around the body of the TCM is decreased. Although further $\xi$ is increased from $\xi = 6$, further change does not occur. Thus, when $\xi$ is increasing, $\mathcal{W}_{TCM}(d)$ is monotonically decreasing to a certain value. This property is also observed for different values of $Z$.

**Remark:** For our Coulomb system, the potential part of the Hamiltonian does not include the masses. Thus, $v_c$ is independent of $\xi$. For the gravitational case, the TCM has the same topology compared with our Coulomb system. But the potential part of the Hamiltonian includes the masses. This makes difference in the behaviour of the flow on the TCM. If $m_1 = 1, m_2 = \xi$, and $m_3 = 1, v_c \sim \sqrt{\xi}$ as $\xi \to \infty$. Therefore, when $\xi \to \infty$, the winding number of $\mathcal{W}_{TCM}(c)$ or $\mathcal{W}_{TCM}(d)$ may not decrease as well as in the case of our Coulomb system. Thus, it is supposed that in the gravitational three-body problem in collinear configuration, the system hardly becomes hyperbolic, namely it always has stable orbits(i.e., tori).

To summarize, when $\xi \to 0$, the orbit on the TCM wind around the body of the TCM infinitely often. When $\xi$ is increased, the number of times that the orbit winds around the body of TCM is monotonically decreasing to a certain value. The latter fact is related to what we examine in the next section.
4. Symbolic dynamics

In this section, we examine the global structure of the Poincaré surface of section by using the associate symbolic dynamics. The Poincaré surface of section is defined as follows: We denote the position on the line \( Q_1 = Q_2 \) in the \((Q_1, Q_2)\)-plane by \( R \), i.e., \( R = Q_1 = Q_2 \). On this line, the momenta \( P_1 \) and \( P_2 \) are specified by new variables \( \theta \) and \( R \).

\[
P_1 = \sqrt{T} \cos \theta + \sqrt{\frac{\xi T}{\xi + 2}} \sin \theta,
\]
\[
P_2 = \sqrt{T} \cos \theta - \sqrt{\frac{\xi T}{\xi + 2}} \sin \theta,
\]

where \( T \) is the kinetic part of the total energy. Our surface of section is the \( (\theta, R) \)-plane where \( 0 \leq R \leq R_{\text{max}}, 0 \leq \theta < 2\pi \) and \( R_{\text{max}} = 2 - \frac{1}{2\pi} \). We denote this plane by \( \mathcal{D} \). We define the map \( \chi \) from the point \( z \in \mathcal{D} \) to the bi-infinite symbol sequence \( n \) which is an itinerary of the orbit started from \( z \) at the time zero.

\[
\chi: \mathcal{D} \to \mathbb{A}^\mathbb{Z}
\]
\[
z \mapsto n = \ldots n_{-2}n_{-1} \cdot n_0n_1n_2 \ldots
\]

We define the map \( \chi^{(+)} \) from the point \( z \) to the semi-infinite symbol sequence \( n^{(+)} \).

\[
\chi^{(+)}: \mathcal{D} \to \mathbb{A}^\mathbb{N}
\]
\[
z \mapsto n^{(+)} = n_{-1} \cdot n_0n_1n_2 \ldots
\]

We also consider the following map \( \Xi_l \) from the semi-infinite symbol sequence to the finite symbol sequence with length \( l + 2 \):

\[
\Xi_l(n_{-1} \cdot n_0n_1 \ldots) = n_{-1} \cdot n_0n_1 \ldots n_l.
\]

Let us introduce

\[
\mathcal{D}_1 = \{(\theta, R) : 0 \leq \theta < \pi, 0 \leq R \leq R_{\text{max}}\},
\]
\[
\mathcal{D}_2 = \{(\theta, R) : \pi \leq \theta < 2\pi, 0 \leq R \leq R_{\text{max}}\}.
\]

There are two symmetry operations on \( \mathcal{D} \). (1) if the orbit starting \( z = (\theta, R) \in \mathcal{D}_1 \) has the symbol sequence \( \ldots m_{-2}m_{-1} \cdot n_0n_1 \ldots \), then \( \ldots n_1n_0 \cdot m_{-1}m_{-2} \ldots \) is a symbol sequence for the point \( (2\pi - \theta, R) \in \mathcal{D}_2 \). (2) if \( m_1m_2m_3 \ldots \) is the future symbol sequence corresponding to the orbit starting at \( (\theta, R) \in \mathcal{D}_1 \) and if \( m_1m_2m_3 \ldots \) is the future symbol sequence corresponding to the orbit starting at \( (\pi - \theta, R) \in \mathcal{D}_1 \), then \( \ldots m_3'm_2'm_1' \cdot n_1n_2n_3 \ldots \) is the bi-infinite sequence corresponding to the full orbit starting at the point \( (\theta, R) \in \mathcal{D}_1 \), where \( m_i' = 1 \) if \( m_i = 2 \) and \( m_i' = 2 \) if \( m_i = 1 \). Thanks to these two symmetry operations, in order to investigate the global structure of \( \mathcal{D} \), it is sufficient to study only the future orbits for the points in \( \mathcal{D}_1 \).

We numerically construct the map \( \chi^{(+)} \) in the following way: we consider the rectangle lattice whose lattice size is \( 1800 \times 1000 \) for \( \mathcal{D}_1 \). For each lattice point \( z_{nm}, 1 \leq n \leq 1800, 1 \leq m \leq 1000 \), we numerically obtained the truncated symbol
sequence $\Xi_60(\chi^{(+)}(z_{nm}))$ by integrating the equations of motion for the Hamiltonian
Eq. (8) using the sixth order symplectic integrator method as mentioned in §2.

As established for celestial problem (Tanikawa and Mikkola, 2000), the following
properties are also true for our Coulomb system:

**Property 4.1:** A trajectory in the $(Q_1, Q_2)$-plane transversely crosses the line
$Q_1 = Q_2$ except at $(\theta, R) = (0, 0)$, if it does at all.

**Property 4.2:** If a trajectory crosses the line $Q_1 = Q_2$ on the $(Q_1, Q_2)$-plane, a
double collision occurs before the trajectory again crosses it.

The proof for the above Properties is the same as in the article (Tanikawa and
Mikkola, 2000).

From the latter Property 4.2, if we put the initial condition $z$ in $D_1$ whose trajectory
crosses the line $Q_1 = Q_2$, then the corresponding orbit has the symbol sequence
$\ldots n_3n_21 \cdot 2n_1n_2 \ldots$, where $n_i \in A$.

The following two things are numerically checked for our Coulomb systems (i.e.,
the case of $(Z, \xi) = (1, 1)$ and the case of the helium) as observed for celestial
problem (Tanikawa and Mikkola, 2000): The plane $D_1$ is divided into two regions of
the points $z$ having $\Xi_1(\chi^{(+)}(z)) = 1 \cdot 22$ and $1 \cdot 21$. Furthermore, it divided into four
regions of the points $z$ having $\Xi_2(\chi^{(+)}(z)) = 1 \cdot 222, 1 \cdot 221, 1 \cdot 212$ and $1 \cdot 211$. This
procedure is repeatedly applied. Then $D_1$ is divided into smaller regions. The second
thing is that the boundaries of regions of different symbol sequences form curves in $D_1$.
It is turned out that these curves are initial conditions of orbits which end in triple
collision. So we call these curves the \textit{triple collision curves}. We denote them by $C_{TC}$.

Figures 5 and 6 depict the triple collision curves $C_{TC}$ for the case of $(Z, \xi) = (1, 1)$
and the case of the helium, respectively. For the case of $(Z, \xi) = (1, 1)$ (Fig. 5), there
is a torus in $D_1$. The simple stable orbits (the torus) may correspond to the Schubart
orbits in celestial problem (Schubart, 1956). Therefore, we call these stable orbits the
S-orbits. In the context of atomic physics, it is usually called the asymmetric stretch
orbit which was found by Simonovic and Rost (Simonovic and Rost, 2001). In Fig 5
the region of the torus (S-orbits) is shown as a triangle area located at $\theta = \frac{\pi}{2}$. For
the point $z$ in this triangle area, it is that $\chi^{(+)}(z) = 1 \cdot (21)^\infty$. In Fig 5 we show the
regions of the points $z$ whose symbol sequence is $\Xi_5(\chi^{(+)}(z)) = 1 \cdot 2n_1n_2 \ldots n_6$, where
$n_i \in A_0 (i = 1, 2, \ldots, 6)$. There are the missing regions of the points $z$ whose symbol
sequence $\Xi_i(\chi^{(+)}(z))$ includes the words 1122 and 2211. Our numerical calculation up
to the word length 15 showed that the inadmissible words are only the words including
the words 1122 and 2211. Note that 1122 and 2211 are also inadmissible words for
the celestial problem (the case of $(Z, \xi) = (-1, 1)$) and other inadmissible words exist
(Tanikawa and Mikkola, 2000). On the other hand, for the case of the helium (Fig 6),
i.e., large $\xi$, there is no torus. Figure 6 shows the regions of the points $z$ whose symbol
sequence is $\Xi_6(\chi^{(+)}(z)) = 1 \cdot 2n_1n_2 \ldots n_6$, where $n_i \in A_0 (i = 1, 2, \ldots, 6)$. In this case,
there is no missing regions (i.e., no inadmissible words). When the symbol sequences
$1.2n_1 \ldots n_l$ with length $l + 2$ are considered, $D_1$ is divided into $2^l$ partitions.
In order to examine the hyperbolicity of the system, we investigate the foliated structure of $D_1$. Using the second symmetry of $D_1$, we construct the triple collision curves whose orbit is started at triple collision in past. We denote the triple collision curves obtained in this way by $C_{TC}$. In Figs. 7 and 8 we depict the triple collision curves whose orbit is started and/or ended at triple collision for the case of $(Z, \xi) = (1, 1)$ and the case of the helium, respectively. Figs. 7 and 8 are constructed from Figs. 5 and 6. It is clearly seen that for Fig. 8 $C_{TC}$ and $C_{tTC}$ transversely cross each other, while for Fig. 7 $C_{TC}$ and $C_{tTC}$ transversely cross each other except near the torus. Since the dynamics of our system is continuous, we expect that $C_{TC}$ and $C_{tTC}$ do not cross the stable and unstable manifolds. For discontinuous system, such as billiard system, this is not the case. In fact, it is numerically confirmed that when $\xi$ is sufficiently large, the triple collision curves $C_{TC}(C_{tTC})$ is parallel to the stable(unstable) manifolds in the Poincaré section for the Poincaré map, respectively. Therefore, Fig. 8 sufficiently large $\xi$ manifests that the dynamics of the helium in collinear eZe configuration is hyperbolic. With some parameter values when the torus exists(for small value of $\xi$), $C_{TC}$ and $C_{tTC}$ do not foliate. In this case, it is observed that the tangency of the $C_{TC}$ and $C_{tTC}$. This may manifest the tangency of the stable and unstable manifolds.

The relationship between the observation in the previous section and the observation in Figures 7 and 8 is unclear at present. Next we clarify this relation by transforming the Poincaré plot in $(\theta, R)$-coordinates into that in $(s, v, w)$-coordinates. The Poincaré surface section in $(s, v, w)$-coordinates corresponding to that in $(\theta, R)$-coordinates is just the plane $s = 0$. The transformation from $(\theta, R)$ to $(v, w)$ is as follows:

$$v = \frac{1}{4\sqrt{2}} (P_1' + P_2') \sqrt{2 - \frac{1}{2Z}} - R,$$

$$w = 4\sqrt{2} \left[ 2\sqrt{2} \left( 2 - \frac{1}{2Z} \right) \right]^{-\frac{1}{2}} s^T A^T p' \sqrt{2 - \frac{1}{2Z}} - R,$$

where

$$P_1' = \cos \theta + \sqrt{\frac{\xi}{\xi + 2}} \sin \theta,$$

$$P_2' = \cos \theta - \sqrt{\frac{\xi}{\xi + 2}} \sin \theta,$$

and

$$p' = \begin{pmatrix} -P_1' \\ P_1' - P_2' \\ P_2' \end{pmatrix}, \quad s = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}.$$ (24)

Figure 9 shows the Poincaré plot of the triple collision orbits in $(v, w)$-coordinates, which corresponds to Figure 7 in $(\theta, R)$-coordinates for $(Z, \xi) = (1, 1)$. $w \geq 0 (w \leq 0)$ corresponds to $D_1 (D_2)$, respectively. First, we note that there is a special solution along the line $s = w = 0$, which starts from the critical point $d$ and ends in $c$. It is given by

$$v = -v_c \tanh \left( \frac{\lambda}{2} (\tau - \tau_0) \right),$$

where
where $\tau_0$ is determined by the initial condition. This solution shows that $W^{s,*}(c)$ and $W^{u,*}(d)$ are degenerated. This type of solution also appears in symmetric gravitational four-body problem (Sekiguchi and Tanikawa, 2002). Second remarkable point is that the triple collision curves $C_{TC}$ and its reversed pair $C^*_{TC}$ accumulate at ten points on the TCM (i.e., $w^2 + W(0)^{-1}v^2 = 1$). Figure 10 for $(Z, \xi) = (1, 1)$ shows one branch of $W_{TCM}(c)$. As shown in Fig.10 these points are the points at which $W_{TCM}(c)$ and $W_{TCM}(d)$ cross the plane $s = 0$. We denote these points by $P_{TCM,r = 0}$. It is easily understood that the number of points of $P_{TCM,r = 0}$ is related to the existence of the tori in the Poincaré surface of section $s = 0$. If the tori exists, its outer most torus has periodic points. These periodic points have the stable and unstable manifolds. Some branches of these stable and unstable manifolds run toward $W_{TCM}(c)$ and $W_{TCM}(d)$. Therefore, the number of the points of $P_{TCM,r = 0}$ is directly related to the period of the periodic points associated to the tori. At the same time, the number of the points of $P_{TCM,r = 0}$ just corresponds to the winding number $N$ of $W_{TCM}(c)$ or $W_{TCM}(d)$ around the body of the TCM as observed in the previous section. In Fig.11 the case of $(Z, \xi) = (1, 7)$ is shown. As the result of the previous section, when $\xi$ is large enough, the winding number of $W_{TCM}(c)$ and $W_{TCM}(d)$ saturates to certain value. In other words, when $\xi$ is large enough, the number of the points of $P_{TCM,r = 0}$ also saturates to certain value which is, in fact, six (i.e., no torus case). Thus, the existence of torus in the Poincaré section $s = 0$ is monitored by the number of points of $P_{TCM,r = 0}$. When $\xi$ is large enough, the triple collision curves $C_{TC}$ transversely cross $C^*_{TC}$. This would be a strong evidence of hyperbolicity of the system with large $\xi$, since it is numerically confirmed that $C_{TC}(C^*_{TC})$ is parallel to the stable(unstable) manifold for the Poincaré map, respectively.

The critical value of $\xi_c(Z)$ at which the winding number $N$ is minimized, is calculated. In Table 1 we summarize the result. For $Z = 1, 2, 3, 4, 5$, the critical value $\xi_c(Z)$ is order of $O(10)$. These critical value is numerically obtained. Thus, these are not true critical values. However, we expect that at these true critical value the unstable manifold of $c$ and the stable manifold of $d$ degenerate. At these critical value $\xi_c(Z)$, the tori disappear. At present, we do not know precise mechanism of this disappearance of the tori, e.g., even whether KAM-scenario is applied or not.

From the above numerical observation, we can state a conjecture. **For the system Eq.(11) with $(Z, \xi)$, there exists the critical value $\xi_c(Z)$ such that for $\xi > \xi_c(Z)$ the system is hyperbolic.**

Since for actual two-electron atom or ions the mass ratio is large, i.e., $m_p/m_e \approx 1840$, this means that the classical dynamics of H$^-$, He, Li$^+$, Be$^{2+}$, ... in collinear eZe configuration is hyperbolic. For infinite mass ratio, it was numerically shown that the symbolic description is complete and the dynamics probably hyperbolic (Bai, Gu and Yuan, 1998).
4.1. The case of \((Z, \xi) = (1, 1)\)

In this subsection, we investigate the detailed structure of the Poincaré surface of section for the case of \((Z, \xi) = (1, 1)\). In this case, there is a torus whose symbol sequence is \(1 \cdot 21212\ldots\) as shown in Figs. 15 and 17. This torus has the periodic points with period 6 as the outermost part. Note that we include the periodic points in \(D_2\) and count the period. These periodic points \(\alpha, \beta, \gamma\) has stable and unstable manifolds. \(\alpha : (\theta, R) = (0.5\pi, 1.385), \beta : (\theta, R) = (0.5292\pi, 1.275),\) and \(\gamma : (\theta, R) = (0.4708\pi, 1.275).\)

From the numerical calculation, one branch of \(W^s(\alpha)\) is equal to one branch of \(W^u(\beta)\). In the same way, one branch of \(W^s(\beta)\) is equal to one branch of \(W^u(\gamma)\) and one branch of \(W^s(\gamma)\) is equal to one branch of \(W^u(\alpha)\). We can construct the stable manifolds of \(\alpha, \beta,\) and \(\gamma\) outside the S-orbits by examining the long orbits with the symbol sequence \(1 \cdot 21212\ldots\). The result is depicted in Fig. 12(a). In Fig. 12(b), we also depict the unstable manifolds by using the second symmetry of \(D_1\). The stable manifolds of \(\alpha, \beta,\) and \(\gamma\) outside S-orbits are basic boundaries of the partitions of \(D_1\).

We further examined the symbol sequence \(\Xi_{60}(z^{(+)m}(z))\) for each \(z_{mn}\) \((0 \leq m \leq 1800, 0 \leq n \leq 1000)\). As a result, \(D_1\) is divided into, at least, ten partitions: \(S, I_i (i = 1, 2, \ldots, 9)\). \(S\) stands for the S-orbits. Other partitions \(I_i (i = 1, 2, \ldots, 9)\) are defined as follows. We examined the symbol sequences \(\Xi_{60}(z^{(+)m}(z))\) along the line \(\theta = 0.2\pi, 0.5\pi, 0.55\pi\) and \(0.7\pi\). For the line \(\theta = 0.2\pi\), we find that the symbol sequences are distributed as it decreases from \(1 \cdot (2)^\infty\) to \(1 \cdot (21)^\infty\) with increasing \(R\). We divide symbol sequences into three groups: \(1 \cdot (2)^\infty, 1 \cdot (2)^n12\ldots, \) and \(1 \cdot (21)^n\ldots (n \geq 2)\). We call the regions with these symbol sequences \(I_7, I_4\) and \(I_1\).

For the line \(\theta = 0.5\pi\), the symbol sequences are distributed as it increases from \(1 \cdot 2(1)^\infty\) to \(1 \cdot (21)^\infty\). We divide symbol sequences into three groups: \(1 \cdot 2(1)^\infty, 1 \cdot 2(1)^n21\ldots, \) and \(1 \cdot (21)^n\ldots (n \geq 2)\). We call the regions with these symbols sequences \(I_8, I_5\) and \(I_2\).

By examining the symbol sequences along the line \(\theta = 0.55\pi\) and \(0.7\pi\), we find that along the line \(R = 1.3\) from \(\theta = \pi\) to \(0.5\pi\), the symbol sequences are distributed as it decreases from \(1 \cdot 21(2)^\infty\) to \(1 \cdot (21)^\infty\) with decreasing \(\theta\). We divide symbol sequences into three groups: \(1 \cdot 21(2)^\infty, 1 \cdot 21(2)^n12\ldots \) and \(1 \cdot (21)^n\ldots (n \geq 2)\). We call the regions with these symbols sequences \(I_6, I_6\) and \(I_3\). Fig. 13(a) shows these partitions of \(D_1\). In Fig. 13(b), the time-reversed partitions by the second symmetry of \(D_1\) are shown with them of Fig. 13(a). In Table 2, the characteristic feature of \(S\) and \(I_i (i = 1, 2, \ldots, 9)\) is summarized.

Next we prepared many points in each partition and checked which partitions they are mapped to. In Table 3, we summarized the transition among the partitions. From Table 3, we drew the diagram of the transitions among partitions in Fig. 14. From this diagram, we know that typical orbits travel around the regions near the torus \((I_1, I_2,\) and \(I_3)\) and/or around the regions in which the orbits feel large instability \((I_4, I_5, I_6)\), and, that in most cases, they escape to the regions \((I_7, I_8, I_9)\) except the S-orbits and non-wandering orbits (probably repellor).
4.2. The case of helium

For the case of helium, Figs. 6 and 8 tell all features of the partitions. The partitions formed by $\mathcal{C}_{TC}$ is, at first sight, expected to be the Markov partitions. If we obtain $\mathcal{C}_{TC}$ using the symbol sequences $1.2n_1 \ldots n_t$, then $\mathcal{D}_1$ is divided into $2^t$ partitions. From numerical observation, there is no inadmissible words. However, it is clear that I and $\tilde{I}$ are removed, since these orbits correspond to fixed points at infinity. The Markov partition should be shaped as parallelepiped. Thus probably, in mathematical rigorous sense, the partitions in our Poincaré section are not the Markov partitions. If we construct the Markov partitions in our Poincaré section, they would be infinite. This reflects the fact that the dynamics of helium atom in collinear eZe configuration exhibits intermittency (Richter, Tanner and Wintgen, 1993, Tanner and Wintgen, 1995, Tanner, Richter and Rost, 2000). The intermittency observed in helium atom in collinear eZe configuration is the behaviour that the electrons are going back and forth between long flight (i.e., almost ionization) and short flight (i.e., successive collisions with the nucleus). This intermittency is due to the existence of the fixed points at infinity. Its behaviour is very similar to hyperbola billiard (Sieber and Steiner, 1990). The transverse crossing of $\mathcal{C}_{TC}$ and $\mathcal{C}'_{TC}$ strongly suggests that the dynamics is hyperbolic.

4.3. The Poincaré plots for other two-electron ions

For the case of the infinite nucleus mass, it was investigated by Bai et al (Bai et al, 1998). It was numerically shown that for $Z \geq 1$, the symbolic description is complete and it suggests that the system is hyperbolic. We now consider the finite mass case. The investigation above does not consider the $Z$-dependence of the dynamics of two-electron atom and ions in collinear eZe configuration. Now in order to strengthen our claim that the dynamics of them is fully chaotic, probably hyperbolic, we calculated the Poincaré plots for thirty atom and ions among the systems $H^-$, He, Li$^+$, ..., Fm$^{98+}$ in collinear eZe configuration. We do not plot them since there is no space. This calculation showed that even though $Z$ becomes large at the order $O(100)$ and then the interaction terms becomes small in Eq. (8), their large mass ratio $\xi$ overcomes the $Z$-dependence to result in the fact that the Poincaré plot is filled by chaotic sea except the escape region and there is no visible torus. These observations strengthen our claim.

5. Experimental aspect

From our observations, we know that the system with small mass ratio qualitatively differs from the system with large mass ratio, namely the existence of stable orbits. This difference would be experimentally observed. A possible candidates are the antiproton-proton-antiproton ($\bar{p}$-p-$\bar{p}$) system, the positronium negative ion(Pr-(e-$\bar{e}$-e)), which corresponds to the case of $Z = 1, \xi = 1$. We neglect relativistic effects, bremsstrahlung and hyperfine interaction. If this system has the bound states, the eigenenergies possesses the effects of the torus. Most convenient analysis is the Fourier
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transform of the density of states for the spectrum with the angular momentum \( L = 0 \), which gives the information on the length and the stability of periodic orbits. For the positronium negative ion, the EBK quantization was done (Simonovic and Rost, 2001). Stable antisymmetric orbit was obtained and was quantized to explain the energy spectrum. From our observation, as a ZeZ configuration, the positive hydrogen molecule \( H_2^+ \) have stable periodic orbits.

In addition, although large \( Z \) two-electron ions are experimentally unrealistic, small \( Z \) two-electron ions serve us the data for the manifestation of our finding (i.e., hyperbolicity (strong chaotic property)). \( H^- \) and He have been already analyzed by the semiclassical method (Gaspard and Rice, 1993, Ezra et al., 1991). Therefore, Li\(^+\) is another candidate. If we change \( Z \), the degree of the intermitency of the dynamics would change (Tanner and Wintgen, 1995). This change may be reflected in the behaviour of the quantum defect of \( H^- \), He, Li\(^+\), Be\(^{2+}\), ....

6. Summary

In this paper, we have investigated the bifurcation in classical Coulomb three-body problem in collinear eZe configuration with finite mass of all three particles. In particular, the main result is that when the mass ratio \( \xi \) is changed, the change of the flow on the TCM is directly related to the existence (or collapse) of the tori. This result suggests that if the mass ratio \( \xi \) is sufficiently large, the dynamics of these system is hyperbolic. This result is consistent with the result (i.e., infinite nucleus mass) by Bai et al. (Bai, Gu and Yuan, 1998). But by our analysis, it was shown that there surely exists a threshold value of \( \xi \) for hyperbolicity. These threshold value is order of \( O(10) \). Therefore, \( H^- \), He, Li\(^+\), Be\(^{2+}\), ... in the collinear eZe configuration is hyperbolic. Since our analysis is based on numerical one, we do not have the proof of this fact. We call for rigorous proof of this result.

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Appendix

In this Appendix, we derive the TCM for our Coulomb systems. Its derivation is completely parallel to the case of celestial problem. The readers are recommended to consult with the article for detail (McGehee, 1974). We start from the Hamiltonian Eq.(4).

\[
\mathcal{H} = T(p) - U(q) = E. \tag{26}
\]
where we removed the dash in Eq. (4). $T(p)$ is the kinetic part of $H$ and $-U(q)$ is the potential part of $H$. The equations of motion in the Cartesian coordinates are given by

$$\frac{dq}{dt} = M^{-1}p,$$

$$\frac{dp}{dt} = \nabla U(q),$$

with the mass matrix

$$M = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \xi & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$  

(27)

We set the center of mass to be zero.

$$q_1 + \xi q_2 + q_3 = 0.$$  

(29)

We set the total momentum to be also zero.

$$p_1 + p_2 + p_3 = 0.$$  

(30)

We consider the transformation from the Cartesian coordinates $(q_1, q_2, q_3, p_1, p_2, p_3)$ with Eqs. (29) and (30) to the McGehee’s variables $(r, s, v, w)$. First, we set

$$r = (q^T M q)^{1/2},$$

$$s = r^{-1} q.$$  

(31)

$r^2$ is the moment of inertia. $s$ represents the configuration of three particles. The triple collision corresponds to $r = 0$. Now we parameterize the variable $s$ by single variable $s$. To do so, we set

$$a = (a_1, a_2, a_3), \quad a_1 = a_2 < a_3$$

$$b = (b_1, b_2, b_3), \quad b_1 < b_2 = b_3$$

(32)

where

$$a^T M a = b^T M b = 1.$$  

(33)

Since we fix the center of mass, namely $a_1 + \xi a_2 + a_3 = 0$ and $b_1 + \xi b_2 + b_3 = 0$, then we have

$$a = \left( -\frac{1}{\sqrt{(1 + \xi)(2 + \xi)}}, -\frac{1}{\sqrt{(1 + \xi)(2 + \xi)}}, \frac{1 + \xi}{\sqrt{(1 + \xi)(2 + \xi)}} \right),$$

$$b = \left( -\frac{1 + \xi}{\sqrt{(1 + \xi)(2 + \xi)}}, \frac{1}{\sqrt{(1 + \xi)(2 + \xi)}}, \frac{1}{\sqrt{(1 + \xi)(2 + \xi)}} \right).$$  

(34)

It is shown that the variable $s$ is parametrized by the variable $s \in [-1, 1]$ as follows (See the article for detail(McGehee, 1974).):

$$s = (\sin(2\lambda))^{-1} [\sin(\lambda(1 - s))a + \sin(\lambda(1 + s))b],$$

(35)

with

$$\cos(2\lambda) = a^T M b = \frac{1}{1 + \xi}.$$  

(36)
Here $\lambda$ is valued as $0 \leq \lambda \leq \frac{\pi}{2}$. We denote the map from $s \in [-1, 1]$ to the configuration $s$ by $S$:

$$S: [-1, 1] \rightarrow \{s : s^T M s = 1, s_1 + \xi s_2 + s_3 = 0\},$$

(37)

Note that $s = -1(s = 1)$ corresponds to the collision of the particles 1 and 2 (2 and 3), respectively. $U(s)$ becomes $V(s) = U(S(s))$

$$= \sin(2\lambda) \left[ \frac{1}{(b_2 - b_1) \sin(\lambda(1 + s))} + \frac{1}{(a_3 - a_2) \sin(\lambda(1 - s))} \right]$$

$$- \frac{1}{Z} \{(b_2 - b_1) \sin(\lambda(1 + s)) + (a_3 - a_2) \sin(\lambda(1 - s))\}$$

(38)

Here we set two matrices $A_1$ and $A_2$

$$A_1 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & -1 & 0 \end{bmatrix},$$

(39)

and define the matrix $A$

$$A = \frac{1}{2 + \xi} A_1 M + \left( \frac{\xi}{2 + \xi} \right)^{\frac{1}{2}} M^{-1} A_2.$$

(40)

Now the variable $s$ is defined as the inverse of Eq. (39).

$$s = S^{-1}(s).$$

(41)

We further set

$$v = r^{\frac{1}{2}} p^T s,$$

$$w = r^{\frac{3}{2}}(1 - s^2)W(s)^{-\frac{1}{2}} s^T A^T p,$$

(42)

where

$$W(s) = 2(1 - s^2) V(s).$$

(43)

We also employ time-transformation two times.

$$dt = r^{\frac{3}{2}} dt', \quad dt' = \lambda(1 - s^2) W(s)^{-\frac{1}{2}} d\tau.$$ 

(44)

In short, the change of variables Eqs. (31), (32), (33), and (42) give the wanted relations, i.e., the energy conservation and the equations of motion. The energy conservation becomes

$$1 - \frac{2w^2}{1 - s^2} = \frac{2(1 - s^2)}{W(s)} (v^2 - 2rE) - 1.$$ 

(45)

The equations of motion become

$$\frac{dr}{d\tau} = \lambda(1 - s^2) W(s)^{1/2} rv,$$

$$\frac{dv}{d\tau} = \frac{\lambda}{2} W(s)^{1/2} \left[ 1 - \frac{1 - s^2}{W(s)} (v^2 - 4rE) \right],$$
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\[
\frac{ds}{d\tau} = w,
\]

\[
\frac{dw}{d\tau} = -s + \frac{2s(1-s^2)}{W(s)}(v^2 - 4rE) + \frac{1}{2}W'(s)(1 - s^2 - w^2)
\]

\[
- \lambda(1 - s^2)\frac{1}{2W(s)^{1/2}}vw. \quad (46)
\]

Finally, we set \( r = 0 \). Thanks to the above transformations, this substitution is meaningful, since the singularities from the double collisions have been removed. From Eqs. (45) and (46), we obtain Eqs. (15) and (16). We can also set \( E = 0 \). Then the same energy relation and the equations of motion are obtained, since \( r \) and \( E \) appear as a term \( rE \). The dynamics of scattering flow for \( E = 0 \) was investigated by Bai et al. (Bai, Gu, Yuan, 1998) for the case of the infinite nucleus mass.

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Figure 1. The triple collision manifold: There are two critical points $c$ and $d$.

Figure 2. The schematic picture of the stable and unstable manifolds of the critical points $c$ and $d$: $\mathcal{W}(c)$ and $\mathcal{W}(d)$ are depicted. $\dim(\mathcal{W}^s(c)) = 2$, $\dim(\mathcal{W}^u(c)) = 1$, $\dim(\mathcal{W}^s(d)) = 1$, $\dim(\mathcal{W}^u(d)) = 2$.

Figure 3. The stable and unstable manifolds of the critical points $c$ and $d$ on the TCM for $(Z, \xi) = (1, 1)$: $\mathcal{W}_{TCM}(c)$ and $\mathcal{W}_{TCM}(d)$. Two circles indicate the positions of two critical points $c$ and $d$.

(a)  (b)

Figure 4. The unstable manifold of the critical point $c$ on the TCM: (a) $(Z, \xi) = (1, 0.1)$, (b) $(Z, \xi) = (1, 6)$.

Figure 5. The triple collision curves $C_{TC}$ for the case of $(Z, \xi) = (1, 1)$: We also plot the torus region (triangle area). The curves are obtained by the symbol sequences with length 7 in future.

Figure 6. The triple collision curves $C_{TC}$ for the case of helium: The curves are obtained by the symbol sequences with length 7 in future.

Figure 7. The triple collision curves $C_{TC}$ and $C^l_{TC}$ for the case of $(Z, \xi) = (1, 1)$: We also plot the torus region (triangle area). These curves are obtained from the data of Fig.5.

Figure 8. The triple collision curves $C_{TC}$ and $C^l_{TC}$ for the case of the helium: These curves are obtained from the data of Fig.6.

Figure 9. The Poincaré plot of the triple collision orbits $C_{TC}$ and $C^l_{TC}$ in $(v, w)$-coordinates for $(Z, \xi) = (1, 1)$. It corresponds to Fig.7.

Figure 10. The Poincaré plot of the triple collision orbits and one branch of the unstable manifold of the critical point $c$ for $(Z, \xi) = (1, 1)$. Three crossing points (including the critical point $c$) where the unstable manifold crosses the Poincaré section $s = 0$ are indicated by squares.
Figure 11. The Poincaré plot of the triple collision orbits $C_{TC}$ and $C_{TC}'$ for $(Z, \xi) = (1, 7)$ in $(v, w)$-coordinates.

(a) (b)

Figure 12. The stable and unstable manifolds of $\alpha$, $\beta$, and $\gamma$ for the case of $(Z, \xi) = (1, 1)$: (a) The stable manifolds of $\alpha$, $\beta$, and $\gamma$, (b) The unstable manifolds (dotted lines) of $\alpha$, $\beta$ and $\gamma$ are also added to (a).

(a) (b)

Figure 13. The partitions in $D_1$ for the case of $(Z, \xi) = (1, 1)$: (a) The partitions in $D_1$, (b) The time-reversed partitions are also added to (a).

(a) (b)

Figure 14. The transition diagram for the case of $(Z, \xi) = (1, 1)$ among the partitions derived from Table 2.
Table 1. The critical value $\xi_c(Z)$.

| $Z$ | $\xi_c(Z)$ |
|-----|------------|
| 1   | 6.4        |
| 2   | 15.0       |
| 3   | 23.5       |
| 4   | 32.0       |
| 5   | 40.4       |

Table 2. The characteristic feature of each partition for $(Z, \xi) = (1, 1)$.

| Partition | Character      | Symbol sequence |
|-----------|---------------|----------------|
| $S$       | S-orbits(torus) | $1 \cdot (21)^\infty$ |
| $I_1$     |                | $1 \cdot (21)^n \ldots (n \geq 2)$ |
| $I_2$     |                | $1 \cdot (21)^n \ldots (n \geq 2)$ |
| $I_3$     |                | $1 \cdot (21)^n \ldots (n \geq 2)$ |
| $I_4$     |                | $1 \cdot (2)^n 12 \ldots (n \geq 2)$ |
| $I_5$     |                | $1 \cdot 2(1)^n 21 \ldots (n \geq 2)$ |
| $I_6$     |                | $1 \cdot 21(2)^n 12 \ldots (n \geq 2)$ |
| $I_7$     | Escape         | $1 \cdot (2)^\infty$ |
| $I_8$     | Escape         | $1 \cdot 2(1)^\infty$ |
| $I_9$     |                | $1 \cdot 21(2)^\infty$ |

Table 3. The transitions among the partitions for $(Z, \xi) = (1, 1)$.

| Transitions                  |
|------------------------------|
| $S \rightarrow S$           |
| $I_1 \rightarrow I_2, I_5, I_8$ |
| $I_2 \rightarrow I_3, I_6, I_9$ |
| $I_3 \rightarrow I_1$        |
| $I_4 \rightarrow I_1, I_2, I_4, I_5, I_7, I_8$ |
| $I_5 \rightarrow I_2, I_3, I_5, I_6, I_8, I_9$ |
| $I_6 \rightarrow I_4$        |
| $I_7 \rightarrow$ Escape     |
| $I_8 \rightarrow$ Escape     |
| $I_9 \rightarrow I_7$        |

Table 3. The transitions among the partitions for $(Z, \xi) = (1, 1)$.