Exploring a Classical Model of the Helium Atom

Tomoyuki Yamamoto¹,*) and Kunihiko Kaneko²

¹Bioinformatica, Utrecht University, Padualaan 8, 3584 CH Utrecht
The Netherlands
and
Department of Mathematics, Hokkaido University, Sapporo 060-0810, Japan
²Department of Pure and Applied Sciences, University of Tokyo
Tokyo 153-0041, Japan

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Classical model of helium atom is numerically studied. The phase space is investigated with several types of configurations. While most of orbits cause autoionization via chaotic transients, three types of tori are found. One type of torus is quantized semiclassically with the EBK scheme. Chaotic motion due to the strong interactions between electrons is always unbounded and leads to autoionization. Complex structure of phase space with tori and unstable autoionizing orbits is studied.

§1. Introduction

After successful quantization of Bohr’s classical model of the hydrogen atom in the early 20th century, Bohr attempted to extend this quantization to helium,¹) with the simple addition of one electron. This attempt failed. Since then, Langmuir,²) van Vleck,³) Landé ⁴) and others tried various models in vain, until Schrödinger completed the basis of quantum mechanics.

The failure of these pioneering semiclassical studies is due to the lack of a full understanding of energy levels and orbits and to the difficulty of calculating trajectories. Those who made these studies adopted only trivial periodic orbits, satisfying trivial symmetry, which turned out to be unstable. As for the correct understanding of quantum-classical correspondence, we had to wait for the work by Gutzwiller,⁵) - ⁷) which shows that all periodic orbits (i.e., including nontrivial ones) have to be taken into account to obtain energy level spacings.

The effort to connect the gap between classical and quantum physics has lead to recent studies in quantum chaos, where systems with low degrees of freedom are often adopted. It is natural to start from well-understood systems, since classical dynamical systems consisting of more than two degrees of freedom are not completely understood. However, the importance of systems with larger degrees of freedom should be emphasized, since it is known that Hamiltonian dynamics with more than two degrees of freedom has different features from the dynamics of low-dimensional systems.

Here we study a classical helium atom with a Coulomb interaction to elucidate various features of the phase space⁸) as a system with three degrees of freedom. As

*) E-mail: ty@math.sci.hokudai.ac.jp
will be seen, chaotic orbits are connected with each other. This leads to the escape of one electron to infinity, while two types of non-trivial tori are found in addition to Kolmogorov-Arnold-Moser type tori. It is hoped that the present study provides a step towards understanding Hamiltonian systems with many degrees of freedom.

§2. Model

We consider only a Coulomb interaction and neglect spins and relativistic effects. Then the Hamiltonian of a many-body system with a Coulomb interaction is described as

\[ H = \sum_i \frac{1}{2m_i} p_i^2 + \sum_{i \neq j} \frac{Q_i Q_j}{r_{ij}} \]

in dimensionless form. Here, \(Q_i\) denotes the charge of the \(i\)-th particle. This system is invariant under the transformation

\[ \frac{L^3}{T^2} = 1, \quad \text{for} \quad r' = Lr, \quad t' = Tt. \]

Here, \(L\) and \(T\) are the scales of length and time, respectively. The mass of an electron is 1, and that of the nucleus is set at 2000 \(\times\) \(Z\) for simplicity.

The model of the helium atom consists of one nucleus and two electrons. The equations of motion are

\[
\begin{align*}
    M\ddot{r}_0 &= \frac{r_1 - r_0}{r_{10}^3} - \frac{r_2 - r_0}{r_{20}^3} - 2e^2, \\
    \ddot{r}_1 &= \frac{-r_1 - r_0}{r_{10}^3} + \frac{r_2 - r_0}{r_{20}^3} - 2e^2, \\
    \ddot{r}_2 &= \frac{-r_2 - r_0}{r_{10}^3} - \frac{r_1 - r_0}{r_{20}^3} - 2e^2.
\end{align*}
\]

The first particle (particle 0) is the nucleus, with +2 charge. \(M\) is the mass ratio of the nucleus to an electron (8000.0). Each electron (particle 1, 2) has a charge of −1.

Here we investigate the two-dimensional case. In other words, all particles move on a plane. We have carried out numerical integration of Eq. (3) with the 4th order Runge-Kutta method and auto-adaptation for the time grid.

Due to high dimensionality, we restricted the investigation to only three types of configurations (CF) of initial conditions. For each condition, we fixed 'electron 2' and varied the initial position and velocity of 'electron 1', as will be described below. Neither the total energy nor the angular momentum is fixed for the initial conditions, since at the first stage, we need a global sketch of the phase space, rather than a detailed picture in a limited area based on conservative variables. The three types of CFs are as follows:

**CF-1** circular form (same direction)

Both electrons are put on the \(X\)-axis. Their initial velocities are parallel to the \(Y\)-axis. The initial distance to the nucleus and the velocity of electron 2 are fixed at \(r_2 = (-1.0, 0.0)\), with \(v_2 = (0.0, -1.0)\). Those of electron 1 are set at \(r_1 = (r_1, 0.0)\), with \(v_1 = (0.0, v_1 > 0)\). Here, the angular momenta of the electrons are in the same direction.
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CF-2 circular form (inverse direction)
Both electrons are put on the same side of the nucleus. Electron 2 is initially at \( r_2 = (1.0, 0.0) \), with \( v_2 = (0.0, 1.0) \), while electron 1 is at \( r_1 = (r_1, 0.0) \), with \( v_1 = (0.0, v_1 > 0) \). Their directions are opposite. This configuration includes the special case in which the total angular momentum is zero.

CF-3 semicircular form
Electron 2 is initially at \( r_2 = (2.0, -0.5) \), with \( v_2 = (0.0, 0.0) \). Electron 1 is at \( r_1 = (x_1, y_1) \), with \( v_1 = (0.0, 0.0) \). Note that the total angular momentum is fixed to zero and only oscillatory motion is allowed. This configuration is similar to Langmuir's semicircular model, but it is not symmetric except in the case \( r_1 = (2.0, 0.5) \).

§3. Results of numerical exploration through the phase space

For the above three configurations, we have investigated the phase space globally with fine resolution. While the energy depends on the initial configuration, it is always kept at a negative value. Due to the strong interaction between electrons, the electrons' orbits are often unstable. For most initial conditions we have seen the autoionization of one of the electrons via a chaotic transient. Here, the "autoionization" is defined as the escape of an electron to infinity.

Ionization is obtained through observation of each electron's energy. We define ionization as the condition in which one of the electrons maintains positive energy for a sufficient watching period (time 10). The ionization time is defined at the time when the watching period is over.

The types of bounded motion we have observed are only regular orbits (i.e., periodic orbits or tori). There is no chaotic bounded motion as far as we have seen — chaotic orbits cause ionization without exception. Generally, ionization takes place within a short period of time (\( \sim 20 \)). It is not due to Arnold diffusion, which requires a very long period of time.

Periodic orbits are not found unless some trivial symmetry is imposed initially. This is because unstable periodic orbits have no measure in the phase space and cannot be found by scanning with a finite resolution.

The tori so far obtained can be classified into the following types. Their stability is confirmed by computing the maximal Lyapunov exponent, which approaches zero asymptotically.

1. double ring (same direction)
   Just like a planetary system, two non-crossing elliptic orbits with different radii exist separately, at a sufficiently large distance. A typical trajectory is shown in Fig. 1, where the two orbits are clearly separated. Their elliptic orbits are distorted by the interaction, and their envelopes are close to centrifugal circles. The condition for the existence of this torus can be estimated by regarding the electron-electron interaction as a perturbation and by examining the non-overlapping of resonances between two elliptic orbits — by following KAM theory: The initial radius \( x_1 \) is regarded as the perturbation parameter when
we assume circular or elliptic orbits. As \( x_1 \) (i.e., the average radius of the orbit) gets close to 1.0 (i.e., \( x_2 \)), the "perturbation" is increased, and the torus region decreases. We have plotted the region where tori exist in Fig. 2 for CF-1 (circular configuration). Here the initial velocity \( v_1 \) is varied by fixing the radius \( (x_1) \). The lower limit of \( x_1 \) is about 1.45. Though the tori have a finite measure in the phase space, the region of existence is not connected. As is seen in Fig. 2, there are holes where tori do not exist. At these 'holes', tori collapse due to the resonance. We have also confirmed the existence of holes by scanning the phase space with a fixed total angular momentum and total energy.

2. double ring (with the inverse direction)
We have also found tori in CF-2 (circular, inverse direction). Since electrons revolve around the nucleus in the opposite direction, their orbits are distorted when they approach in a head-on collision course. In spite of such strong interference, there are tori with strange shapes. As two orbits become close, they are deformed strongly; the outer electron forms loops. In Figs. 3 and 4, we show the transition of the deformation of tori by changing \( x_1 \) of CF-2. The direction of the loop is changed as \( x_1 \) decreases (compare Fig. 5 and Fig. 6).

3. braiding
In CF-1 (circular, same direction), no double ring torus exists for \( x_1 < 1.45 \), where a strong interaction breaks the tori. However, surprisingly enough, there are tori with strange shapes, which we call "braiding tori". The trajectory is shown in Fig. 7, where two electrons rotate in the same region. Their shape is shown in Fig. 8. This torus exists at about \( x_1 \in [1.38, 1.45] \). Only around the upper limit \( (x_1 = 1.45) \) to both the braiding and the double ring tori exist for different regions of initial velocity \( v_1 \).

Though this torus is sustained by the delicate phase relationship between two electrons, it exists within a finite region in phase space.
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Fig. 3. Orbits of two electrons up to time 112, starting from the initial conditions for CF-2: \((r_1, v_1) = (3.0, 0.50)\). No deformation can be seen.

Fig. 4. Orbits of two electrons up to time 211, starting from the initial conditions for CF-2: \((r_1, v_1) = (3.0, 0.42)\). The outer electron loops outward.

Fig. 5. Orbits of two electrons up to time 872, starting from the initial conditions for CF-2: \((r_1, v_1) = (3.0, 0.40)\). The shape of the loops is strongly deformed. Similar orbits were found by Yuan.

Fig. 6. Orbits of two electrons up to time 460, starting from the initial conditions for CF-2: \((r_1, v_1) = (3.0, 0.34)\). The looping direction becomes inward.

4. semicircular

In this case, we have adopted the initial semicircular configuration CF-3, which restricts the total angular momentum to zero. Under this condition, oscillatory motion is often observed. Since initial velocities are restricted to zero, the starting point gives the turning point. If the initial conditions are symmetric with respect to the \(Y\)-axis, there is a trivial periodic orbit with two modes of 1 : 1 resonance — the periodic orbit which Langmuir studied. In the neighborhood of Langmuir’s orbit, there is a type of torus which is originally found and quantized by Noid et al. Though the envelope of the trajectory is symmetric, the trajectory itself is not symmetric.

While Langmuir’s torus is locked with a 1 : 1 resonance, we have found some tori with other locking rates. A 6:1-locking torus is shown in Fig. 10. The tori
Fig. 7. Orbits of braiding torus up to time 90, starting from the initial conditions for $\text{CF-1}:(r_1, v_1) = (1.40, 0.86)$. The two electrons rotate within the same region.

Fig. 8. Orbits of braiding torus up to time 90, starting from the initial conditions for $\text{CF-1}:(r_1, v_1) = (1.40, 0.86)$. The trajectory is plotted by varying the density of loci by the interval of time 0.7. The two arrows indicate the starting points of the two electrons.

Fig. 9. Trajectory of a semicircular torus with 1:1 locking, starting from the initial conditions for $\text{CF-3}:(x_1, y_1) = (2.00, 0.3475)$.

Fig. 10. Trajectory of semicircular torus with 1:6 locking up to time 232, starting from the initial conditions for $\text{CF-2}:(x_1, y_1) = (2.50, 0.40)$. Note that $L = 0$.

with other locking rates will be found in their neighborhood. In this context, the FPA (frozen-planet approximation) periodic orbit studied by Richter and Wintgen\textsuperscript{10,11} is regarded as the extreme case of 1:0 locking.

In fact, the tori are difficult to observe, and most of the area of phase space is occupied by the ionizing orbits. The area where a double ring torus exists is shown in Fig. 2. The tori occupy only a small area of the whole phase space, although they occupy the largest volume among the tori. Other tori (e.g. of the braiding type) occupy a much smaller volume, as is shown in Fig. 11. While ionizing orbits are usually neglected in semiclassical theory, they are important to understand the structure of phase space, as is discussed below. It should be noted that non-trivial
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Fig. 11. Ionization time ($T_{out}$) with $v_1$ at CF-1. $r_1 = 1.45$. The regions where two types of tori exist are also indicated by arrows. Note that the plot outside the zone is not zero — ionization takes place at the lower limit of the ionization time, which is defined by the watching period (see §3).

periodic orbits have not been found in this system so far, although their existence might be expected. They are difficult to find in numerical searching processes with finite resolution. We have obtained only trivial periodic orbits whose shapes are defined by symmetry with respect to certain axes.

Now, let us investigate the ionizing orbits in more detail. In general, the ionizing orbits can roughly be classified into two phases. One is the chaotic phase, when two electrons remain in the neighborhood of the nucleus, and the electrons’ orbits are chaotic due to the strong interaction between them. The other is the ballistic phase, when one of the electrons is kicked out of the neighborhood of the nucleus by taking an elliptic, parabolic, or hyperbolic orbit. Then we have a two-body interaction between the outgoing electron and the ion (i.e., the nucleus and the other electron). Thus the orbit is regular in this phase. By increasing the energy of the outer electron, its orbit is changed from an elliptic orbit to a hyperbolic orbit via a parabolic orbit.

At the end of the ballistic phase, the outer electron that returns to the ion suffers a collision. When the kicked electron has a positive energy, ionization takes place. The ionizing orbit can be regarded as a scattering process, when we focus on the interaction between the outer electron and the ion. To see this point, we have plotted the ionization time ($T_{out}$) vs $v_1$ for CF-1, in Figs. 11 and 12. Each plot is classified into two regions. In the first region, the ionization time is kept constant, as shown. In such plateau regions, ionization takes place quickly. The ionization takes place at the first collision, as is shown in Figs. 12(a)–(f).

We should note that the orbits within this region are essentially given by Rutherford scattering, since the collision takes place only once, and the interaction between electrons rapidly decreases after the ionization. For example, in Figs. 12(b)–(d),
Fig. 12. The transition of orbits outside of a zone. $x_1 = 1.02$ at CF-1. The initial velocities ($v_1$) are: (a) 0.64, (b) 0.71, (c) 0.80, (d) 0.90, (e) 1.01, (f) 1.10, as is shown on the above $T_{\text{out}}$-$v_1$ plot. The numbers correspond to the indices of the electrons. Note that (b, c, d) and (e, f) have common topologies.

the electron on the left side (electron 2) is kicked out and these three orbits have a common topology. A continuous transition is shown. Similarly, in Figs. 12(e) and (f), the right electron (electron 1) is kicked out. It is also important to note that the topologies of the orbits of two neighboring plateau regions (e.g., between Figs. 12 (a) and (b), or between 12(d) and (e)) differ.

Besides the plateau regions, there are regimes with rugged structure, which we call "zone structure". A large zone is shown in Fig. 11. Roughly speaking, a zone seems to be a set of many peaks. In Fig. 11, most of the peaks are parabolic orbits, unless it is specified as a torus in the figure. While the existence of the peak points at the top of the vertical axis implies no ionization, most of them are parabolic orbits—indeed, the existence of tori is rare. Each zone is bounded by peaks (i.e., parabolic orbits) and its bottom has a U-shaped envelope (see $v_1 \sim [0.55, 0.6]$ and $[1.1, 1.25]$ in
Fig. 13. The boundary of zone. $x_1 = 1.02$ at CF-1, with the change of $v_1$ as (a) 0.406, (b) 0.45, (c) 0.55, (d) 0.64 (parabolic orbit and boundary of the zone), (e1) and (e2) 0.66 (inside zone). While one of the electron is kicked out up to time 10 (e1), it returns to make a collision again (e2).

Fig. 11). The latter feature implies a “semi-continuous” transition of the ionization time. In contrast to the plateau regime, ionization takes place not at the first collision but at the second collision. As $v_1$ is varied towards the inside of zone, the period of an elliptic orbit (at the ballistic phase) and the ionization time become shorter, and the U-shaped envelope of the ionization time is realized. In Fig. 13, we show the orbits around the edge of a zone.

However, we should note that there are many peaks within the zone and the U-shape is given only as an envelope. In fact, the orbits within the zone are strongly dependent on the initial conditions, as in chaotic-scattering processes. For example, at many peaks in the U-shaped area (see Fig. 11, $v_1 \sim [1.1, 1.25]$), ionization does not take place at the second collision. Then, another collision can take place, and another level of zone is produced. Within each zone, many “micro-zones” exist, as is shown in Figs. 11 and 12. While the shapes of the orbits become complicated, the topology of the orbits within each micro-zone is the same, as is shown in Fig. 12. Thus, a self-similar structure of zones is often seen in the phase space of a Hamiltonian system. Such a structure is known in the scattering process (e.g., Ref. 12)). However, to construct a symbolic coding system for the zone structure is a difficult problem.

Finally, it is important to note that the outgoing electron can be exchanged at the collision. Then, a symbolic coding of our model (as is done in Ref. 13)) is difficult, since we must deal with two particles at once, and the possible number of codes increase rapidly. Moreover, torus regions exist within zones, while the shapes of tori have a close relation to the neighboring ionizing orbits. The tori are regarded as the orbits which keep colliding forever, and the length of their symbolic codes diverges.
§4. Application of semiclassical theory

Following the correspondence principle between quantum and classical physics, one can expect the existence of the energy levels corresponding to the tori we have discovered. At what energy can we expect the new levels corresponding to the braiding tori? To address the question, we calculate the action integrals of the braiding tori to apply semiclassical quantization with the EBK-scheme.\(^{14)-16}\)

In Fig. 14, the phase portrait of a braiding torus in hyperspherical coordinates is shown, which is defined as follows:

\[
\theta = r_1 r_2, \tag{4}
\]

\[
\alpha = \arctan \frac{r_1}{r_2}, \tag{5}
\]

\[
R = \sqrt{r_1^2 + r_2^2}. \tag{6}
\]

Here, \(\theta\) is the angle between \(r_1\) and \(r_2\). The origin of the coordinates is the center of mass. Since hyperspherical coordinates disregard the total angular momentum and focus on only the angular relationship between electrons, it is convenient to see the topology of two electron’s orbits of a braiding torus. In contrast to the orbit in Cartesian coordinates (Fig. 8), the precession is eliminated here. This makes it easier for us to grasp the phase space structure. We should note that the magnitude of \(\theta\) is \(4\pi([-\pi, 3\pi]\) in the figure), since the inner electron revolves twice while the outer one revolves once. There are crossing points of the \(\alpha - \dot{\alpha}\) and \(R - \dot{R}\) plane due to the exchange of the inner/outer relation of the electrons.

While the EBK scheme gives a one-to-one correspondence between one classical orbit and a set of quantum numbers, it is possible to quantize a set of tori at once since tori form “islands” with a finite measure, as is shown by KAM theory.\(^{17)-19}\) Within an island, tori exist densely around the elliptic points like concentric circles. Those tori have common topologies and their action integrals (i.e., areas of Poincaré section in the appropriate surface) vary almost continuously when the perturbation is small. Then we can estimate the range of quantum numbers by scanning the action integral of this island of a braiding torus.

We have obtained the elliptic point at the center of the island and estimated the range of the island through numerical scanning, as described below.

First, we choose Poincaré surface of section as a four-dimensional manifold at \(\theta = \pi\) (see Fig. 15). By slicing this manifold at the central elliptic point of the island, we obtain the one-dimensional Poincaré section as the path of the action-integration. We have obtained the calculated central elliptic point by applying a Newtonian-method like iteration, taking the center of the Poincaré section as the next initial condition repeatedly. The elliptic point, thus obtained, is \((\dot{\alpha}_0, \dot{R}_0) = (-1.40 \times 10^{-4}, 3.60 \times 10^{-4})\). Here the planes of sections are given by

\[
\dot{\alpha} = \dot{\alpha}_0, \tag{7}
\]

\[
\dot{R} = \dot{R}_0. \tag{8}
\]
Then, we scan the island from the elliptic point to the outside. In Figs. 16 and 17, several examples of Poincaré sections are shown. Since their areas are small compared with the action integral along the trajectory, the actions along the projected plane are also very small.

The shapes of tori are deformed as the orbit goes far from the elliptical point. The deformation (as well as a finer structure of islands) is generally expected in a Hamiltonian system. Since this deformation is slight and the topologies of orbits are identical, it is neglected within the semiclassical theory.

The scanning path is defined by fixing the total energy. The total angular momentum is not conserved during the above described scanning sequence. Although the equation of motion is scalable (see Eq. (2)), the dimension of the scaling factor differs from that of the energy or of the angular momentum. Then the scanning path is defined by the parameter $dx$:

$$x_1 = x_{1c} + dx,$$

$$x_2 = x_{2c},$$

$$v_1 = \sqrt{2 \left( \frac{2}{x_{1c}} - \frac{2}{x_1} + \frac{1}{x_{1c} + x_{2c}} - \frac{1}{x_1 + x_2} \right) + v_{1c}^2},$$

$$v_2 = v_{2c}. $$
Fig. 15. An example of Poincaré section at $\theta = \pi$. Since the number of degrees of freedom is reduced to four, the projection to two-dimensional planes from four-dimensional manifold is given. Projections in the four directions are shown.

Fig. 16. Computed Poincaré sections by slicing with $\dot{R} = \dot{R}_0$. Sections obtained from different initial conditions are imposed. The arrow indicates the obtained elliptic point (closed diamond).

Fig. 17. Computed Poincaré sections by slicing with $\alpha = \alpha_0$. Sections obtained from different initial conditions are imposed. The arrow indicates the obtained elliptic point (closed diamond).
Here, $x_{1c}$, $v_{1c}$, $x_{2c}$ and $v_{2c}$ are taken from the central elliptic point.

Now, we define the paths of action-integration as

1. $S_\theta$: trajectory subtracting the contributions of $S_\alpha$ and $S_R$.
2. $S_\alpha$: Poincaré section of $\alpha-\hat{\alpha}$.
3. $S_R$: Poincaré section of $R-\hat{R}$.

Each path is given a set of quantum numbers ($n_\theta$, $n_\alpha$ and $n_R$, respectively).

Then, it is possible to assign quantum numbers to action integrals obtained numerically. The actions ($S_\theta^{th}$, $S_\alpha^{th}$ and $S_R^{th}$) and the quantum numbers have the following relations:

$$S_\theta^{th} = 2\pi \left( n_\theta + \frac{\beta_\theta}{4} + \omega_\alpha \left( n_\alpha + \frac{\beta_\alpha}{4} \right) + \omega_R \left( n_R + \frac{\beta_R}{4} \right) \right),$$  \hspace{1cm} (13)

$$S_\alpha^{th} = 2\pi \left( n_\alpha + \frac{\beta_\alpha}{4} \right),$$  \hspace{1cm} (14)

$$S_R^{th} = 2\pi \left( n_R + \frac{\beta_R}{4} \right).$$  \hspace{1cm} (15)

$\omega_\alpha$ and $\omega_R$ are the winding numbers on Poincaré sections. $\beta_\theta$, $\beta_\alpha$, $\beta_R$ are the Maslov indices. Their values are 2 for all paths of our braiding tori. We should note that the action values are rescaled together by rescaling the system by Eq. (2). Thus, one can rescale the values of the actions from those obtained numerically. In particular, we can rescale the system so that the minimal action can satisfy the condition for the zero-point oscillation, as is described below. By doing so, the smallest of the actions is given by the zero corresponding quantum number, while the largest one may require a huge number of quantum numbers.

The actions are calculated from the trajectories (for $S_\theta$) and Poincaré sections (for $S_\alpha$ and $S_R$). In contrast with $S_\theta$ about 10, other integrals are very small, as is expected from Figs. 16 and 17.

From the area of the largest sections of existing tori, $S_\alpha$ and $S_R$ are estimated to be on the order of $10^{-5}$ (see also Table I). Thus we neglect the contribution of $S_\alpha$ and $S_R$ in Eq. (13). Hence we need to compute only $S_\theta$, taking a real trajectory on our torus. Near the elliptic point, the tori are approximated by an ellipse. For each Poincaré projection onto the ($\alpha, \hat{\alpha}$) and ($R, \hat{R}$) space, we approximately obtain ellipses. We denote the major axis of the ellipse by $\delta_\alpha$ ($\delta_R$) and the minor axis by $\delta_{\hat{\alpha}}$ ($\delta_{\hat{R}}$). For small radii, the actions are then evaluated as

$$S_\theta = S_0,$$  \hspace{1cm} (16)

$$S_\alpha = \frac{\pi}{2} \delta_\alpha \delta_{\hat{\alpha}},$$  \hspace{1cm} (17)

$$S_R = \frac{\pi}{2} \delta_R \delta_{\hat{R}}.$$  \hspace{1cm} (18)

Here, $S_0$ is the action integral of the real trajectory of the elliptic point, which is obtained by summing its action numerically. The values $\delta_\alpha, \delta_{\hat{\alpha}}, \delta_R$ and $\delta_{\hat{R}}$ are estimated from the computed Poincaré sections (Figs. 16, 17 and Table I). Here we approximate the action integral by this ellipse form up to the region where the shapes of sections are deformed.
Here we should note that each action must satisfy a zero-point oscillation to assign a quantum number. Since $S_{\alpha}$ and $S_R$ are small, we rescale the coordinates by Eq. (2) to increase the actions up to the minimum values of $S_{\alpha}^{th}$ and $S_R^{th}$ ($S_{\alpha}^{th} = \pi$ for both). Then, the maximum value of the smallest action ($S_{\alpha}$) gives the lowest quantum number. These maximal values are obtained from the torus with the largest Poincaré section we have found, which are shown in Table I. Since the scaling does not change the ratio among the actions, $S_{\theta}$ is also scaled upward. Then, the minimum value of the largest quantum number ($\ell_0$) is estimated as $\sim 10^6$. A state with such high quantum number has not yet been observed experimentally.

The total angular momentum ($L$) is also quantized. From the above result, $L$ must be rescaled up to $\frac{\pi}{S_R}$, and it is estimated as $\sim 10^5$. The Langer correction $^{21,22}$ is neglected, since it is negligible compared with this large value.

§5. Discussion

While we regarded an island as a dense set of tori in the last section, there are much finer structures. Generally, an island has many micro-islands within it. Thus there can be many elliptic points and tori other than the central one. Although the existence of such complex structure is known in classical dynamics, it is thought to be less important in semiclassical theory: The action integral from minor islands within an island corresponds to higher quantum levels, since the Poincaré sections of such small tori have only small action integrals. Then they do not influence the result. Although their shapes can be different from that of the major island (i.e., a braiding torus), such tori with different shapes were not obtained here.

There exist many hyperbolic points within an island. They can lead an electron to cause autoionization and form 'holes' — the region in which autoionization takes place — within a torus region, as is shown in Fig. 2. While holes are difficult to observe for our braiding tori, there are some around the edge of an island. Thus one might suspect that tori may not exist in the phase space corresponding to the estimated quantum energy level, and we might need much higher energy to observe the energy level.

However, if we take into account the localization due to quantum effect, tori are stabilized as long as the Planck constant is finite. Then the quantum correspondents of tori are expected to exist at a much wider range, and the existence of hyperbolic points do not destroy the quantum state around the energy level. Furthermore, we may extend our quantum states to lower lying states by applying some extrapolation method. $^9$

While we have found several types of tori, it is natural to ask if there are other types of tori. Though the existence of tori of a semicircular type with a variety of locking ratios is rather trivial, a braiding torus represents a nontrivial type. Also,
other nontrivial types of tori may exist. However, the searching process for such tori should require a huge computation. Since a braiding torus is sustained by a delicate phase relationship, it exists only within a small region. Discovery of other tori with strange shapes requires massive computational power or a highly optimized algorithm.

Though the existence of a torus with a strange shape is interesting in the study of classical dynamics, its contribution to quantum mechanics may be minor. Since the measure of such tori in phase space is expected to be small as long as we assume a braid-like torus, the ratio of actions is thought to be large. Hence their corresponding quantum states must have rather large quantum numbers, as mentioned in the last section, and they may be very difficult to observe.

The quantum number corresponding to such a torus depends on the volume it occupies. It is possible to make an estimation of the corresponding quantum number from the volume of the tori. According to our results, we assume a maximal action \( S_0 = 10 \) and minimal action \( S_1 = 1 \times \delta^2 \). Here, \( \delta \) is the radius of Poincaré section, assuming a circle. The maximum value of \( \delta (\delta_{\text{max}}) \) can be regarded as the volume the tori occupy. We can expect to find this torus by scanning the initial conditions with the resolution of \( \delta_{\text{max}} \). On the other hand, the action must be rescaled to satisfy the zero point oscillation of \( \pi/2 \). Then the lower limit of the maximum quantum number is given by

\[
n = \frac{S_0}{S_1} = 0.1 \times \delta_{\text{max}}^{-2}.
\]

Solving with \( \delta \), we obtain

\[
\delta_{\text{max}} = \sqrt{\frac{0.1}{n}}.
\]

Thus we need \( \delta_{\text{max}} \approx 0.31 \) for \( n = 1 \) and \( 0.031 \) for \( n = 100 \). In this sense, a rather rough scan is sufficient to obtain a torus corresponding to a small quantum number, because the area of island is given by \( \delta_{\text{max}} \).

We have also studied gravitational systems by adopting only an attractive interaction. Taking the solar system in mind, we used one heavy particle (mass \( M \)) and several light particles (mass \( m \)). Even in a gravitational system, we have seen the escape of chaotic orbits when the mass ratio \( (M/m) \) is small (about 10). Even when the ratio is much larger, as in our solar system, this escape is quite common. For example, when the distance between two ‘planets’ is not large, one of them is easily kicked out to infinity. A sufficient distance between planets is required for the stability of our solar system, similar to the situation regarding our double ring and semicircular tori which exist only when two electrons are distant. The sudden escape of chaotic orbits is a generic feature of \( 1/r^2 \)-force systems.

§6. Conclusion

Through this study, we have seen several types of tori and ionization of chaotic orbits. In phase space, the regular region of tori and the chaotic region of ionizing
orbits are mixed in a complicated manner, as is characterized by the zone structure. We have also calculated the action integral of the braiding torus to estimate its corresponding quantum number. The maximum quantum number is extremely large, due to the large ratio among the actions. Though our result is not comparable to known quantum states, it will be useful when one considers the correspondence between classical orbits with finite angular momentum and quantum states. Also, such highly excited level as ours may be observed in interstellar material. Another interesting possibility is the search for quantum number sequences that reach the energy level we have obtained. While direct correspondence is unknown, it may be possible to find corresponding series of quantum numbers when we apply extrapolation via group-theoretical quantum numbers, as is carried out in Ref. 9).

Autoionizing chaotic orbits occupy the largest part of the phase space. This result is thought to raise a problem concerning semiclassical theory, most of which focuses only on either unstable periodic orbits or tori. By summing up all unstable periodic orbits, the semiclassical energy level is estimated there using Gutzwiller’s trace formula. 7) However, in any neighborhood, there are autoionizing orbits which have a finite measure (or occupy almost all the phase space). They also exist even in the neighborhoods of tori. It is not yet clear whether if we can justify neglecting all ionization orbits adopted in the semiclassical theory based on the unstable periodic orbits.

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