Helium Atom as a Classical Three-Body Problem

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(Received 9 November 1992)

The classical three-body problem of the helium atom is numerically studied. For most initial conditions, orbits show chaotic transients until one of the electrons always escapes to infinity, leading to autoionization. For the remaining parts of initial conditions, several types of stable quasiperiodic motions (on tori) are found, which have a finite measure in the phase space. This discovery enables us to treat semiclassically a strongly correlated electronic system.

PACS numbers: 31.20.Tz, 03.20.+i, 05.45.+b

Gravitational three-body problems have been one of the most important examples in nonintegrable Hamiltonian systems. A three-body problem with a Coulomb interaction, on the other hand, is of importance not only in this context but also as a semiclassical approach to a quantum problem. In the 1920s, some of the pioneers in quantum mechanics struggled to make a classical model of the helium atom [1]. Their approach is based on the Bohr-Sommerfeld semiclassical quantization of periodic orbits with special symmetry. These orbits include Bohr's circular model [2], Langmuir's double circle and semicircular models [3], and Landé's model [4], as are reviewed in [1]. Their efforts completely failed, however, mainly due to the instability of their periodic orbits. As will be shown, these orbits show a chaotic behavior by any slight change of initial conditions, and lead to an escape of one electron, implying "autoionization."

Since then, semiclassical quantization schemes have been developed for torus motion according to Einstein [5,6], and for chaotic orbits by Gutzwiller [7]. In a classical helium atom, all chaotic orbits lead to autoionization as will be shown. Thus we focus on the search for stable torus motion, since it is the only possible classical correspondence in the helium atom. Indeed we will report discovery of novel types of tori with strong correlation between electrons.

Classically the dynamics of helium atom (with one nucleus and two electrons) is described by the following dimensionless form:

$$\begin{aligned} M\ddot{\mathbf{r}}_0 &= \frac{\mathbf{r}_1-\mathbf{r}_0}{r_{10}^3}2e^2+\frac{\mathbf{r}_2-\mathbf{r}_0}{r_{20}^3}2e^2, \\ \ddot{\mathbf{r}}_1 &= -\frac{\mathbf{r}_1-\mathbf{r}_0}{r_{10}^3}2e^2+\frac{\mathbf{r}_1-\mathbf{r}_2}{r_{12}^3}e^2, \\ \ddot{\mathbf{r}}_2 &= -\frac{\mathbf{r}_2-\mathbf{r}_0}{r_{20}^3}2e^2-\frac{\mathbf{r}_1-\mathbf{r}_2}{r_{12}^3}e^2. \end{aligned} \tag{1}$$

Here, the first particle (particle 0) is a nucleus, with $+2e$ charge. M is the mass ratio of nucleus to electron (8000.0). Two electrons (particles 1,2) have -1 charge. Equation (1) is invariant under the transformation $t\to Tt, \mathbf{r}\to L\mathbf{r}$ for $T^2/L^3=1$. (Here, T and L are units of time and length, respectively.) Thus the same trajectory (except the scale change) exists for any (negative) energy, by the above scale transformation. Torus orbits to be discussed exist at any energy in classical mechanics through the above transformation.

We restrict our problem to a two-dimensional case only. By choosing a frame with a center of mass, our system has 4 degrees of freedom. Because of the conservation of energy and angular momentum, the degrees of freedom is reduced to 3, with a six-dimensional phase space. We have carried out numerical integration of Eq. (1) with fourth order Runge-Kutta method and autoadaptation for the time grid. Since the dimension of the phase space here is rather high, it is almost impossible to examine all possible trajectories. In the present Letter we study the following types of initial configurations in detail [8]: (1) Circular form (same direction)—Initial distance to nucleus and velocity of electron 2 are fixed at $\mathbf{r}_2=(-1.0,0.0)$, $\mathbf{v}_2=(0.0,-1.0)$. Those of electron 1 are set at $\mathbf{r}_1=(r_1,0.0)$, $\mathbf{v}_1=(0.0,v_1>0)$. (2) Circular form (inverse direction)—Both electrons are put on the same side of the nucleus. Electron 2 is fixed at $\mathbf{r}_2=(1.0,0.0)$, $\mathbf{v}_2=(0.0,1.0)$, while the other one is set at $\mathbf{r}_1=(r_1,0.0)$, $\mathbf{v}_1=(0.0,v_1>0)$ [9]. (3) Semicircular form—Electron 2 is fixed to $\mathbf{r}_2=(2.0,0.5)$, $\mathbf{v}_2=(0.0,0.0)$. Electron 1 is $\mathbf{r}_1=(x_1,y_1)$, $\mathbf{v}_1=(0.0,0.0)$. Note that the total angular momentum is zero.

For a wide range of initial conditions, we have seen the autoionization, that is the escape of one of the electrons to infinity. Indeed, all orbits with irregular motion (chaotic transients) lead to autoionization, as far as we have checked. We believe that this is true for all chaotic trajectories, since all chaotic orbits are believed to be connected in a high-dimensional Hamiltonian system by the Arnold diffusion.

The only remaining possible trajectories keeping the stability are tori. Through numerical integration, we have discovered three types of tori. We have confined the quasiperiodicity of these orbits by the Lyapunov exponent asymptotically going to zero, as well as through the time series and Poincaré plots of orbits. The torus motion here is confined within a finite region of phase space, not ionized spontaneously. By a small change of initial configurations, the torus motion still remains. The torus motion

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has a finite measure in the phase space. The tori so far discovered are classified into the following types.

Type A: double ring— KAM *torus type.*— If two electrons are distant, with the orbits close to two ellipses, the dynamics is approximated by two Kepler motions for the $+2e$ nucleus (for the inner electron) and for the $+e$ charge (for the outer one). The ratio between the two radii (small to large one) plays the role of perturbation parameter in the Kolmogorov-Arnold-Moser (KAM) theory. As the perturbation grows, shapes of remaining tori are distorted. In the type-1 configuration, tori exist, for example, $r_1 \gtrsim 1.45$ for $v_1 \approx 0.95$. Closures of orbit of each electron are concentric circles. Here we note that some tori remain even with a strong interaction between electrons. The existence of tori makes it possible for us to take fully into account the interaction between electrons, without referring to a one-body wave function as in the usual variational trial one.

Tori of this type also exist even when the angular momenta of the two electrons are opposite, as are obtained with the use of the type-2 configuration, for example, around $(r_1,v_1)=(3.0,0.40)$. When the ratio between two radii is far from unity, the orbit is again approximated by two ellipses modulated quasiperiodically. As the two electrons get closer, the torus orbit is deformed more strongly, as shown in Fig. 1. When the outer electron starts looping, the inner one changes its direction to conserve the total angular momentum, and vice versa.

Type B: Braiding.— When the distances of two electrons from a nucleus are close, a novel type of stable orbit is found starting from some examples of type-1 configuration (see Figs. 2 and 3). This type of torus exists around $1.39 \lesssim r_1 \lesssim 1.45$, and $v_1 \approx 0.86$. Here the closure of orbits are identical for each electron. Only the phases of two orbits are different. Two existence probabilities for each electron (obtained by a long time sampling) agree. In the term of quantum mechanics, two electrons lie on the same level. This type of torus has again a finite measure in the phase space, and can be semiclassically quantized by suitably choosing their positions. Here two electrons must satisfy a delicate phase relationship (see Fig. 3); otherwise one of the electrons is kicked away to infinity. In each orbit an electron revolves twice in the inner side, while the other revolves once at the outer circle, before they exchange their position.

Existence of this type of torus is not expected from a perturbative picture based on a two-body problem. The stability of the torus is sustained by the strong interaction between electrons.

Type C: Semicircular.— Here we search for a torus in a strongly coupled regime (the ratio of radii is close to one), by choosing the initial velocity to zero, so that the angular momentum vanishes (configuration 3). We have again found torus motion close to the form of Langmuir's periodic orbit [10], e.g., $x_1=1.95$, $y_1=0.50$. The main difference here is the lack of symmetry. In Langmuir's periodic orbit the symmetry condition $r_{1x}=r_{2x}, r_{1y}=-r_{2y}$ is imposed, while in our case two electrons are asymmetric against the nucleus. Indeed, the periodic orbit of Langmuir is unstable by a slight (asymmetric) perturbation, while our torus exists at a finite distance from the periodic orbit. The torus motion here consists of the oscillatory mode similar to Langmuir's model and librations around it. In this case, the ratio of frequency of oscillations of two electrons is roughly 1:1. By changing the initial velocity, we have also observed a torus with a different phase relationship. An example with 6:1 locking is shown in Fig. 4 [11].

For configuration 1, we have checked initial conditions in the rectangular region; $r_1 \in [1.0,2.0]$, $v_1 \in [0.1,1.6]$.

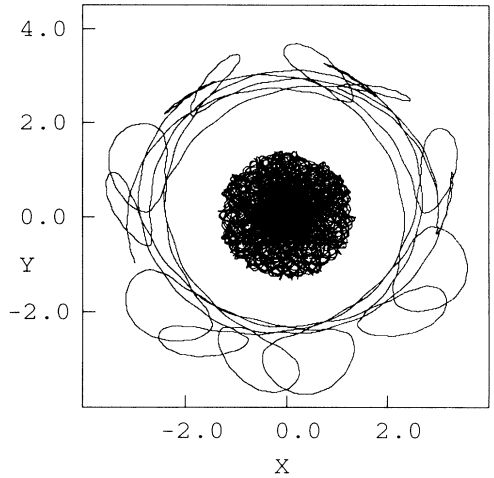

FIG. 1. Double ring torus (inverse direction). Orbits of two electrons are shown for $0 \le t \le 601$, using type-2 configuration with $(r_1,v_1)=(3.00,0.40)$.

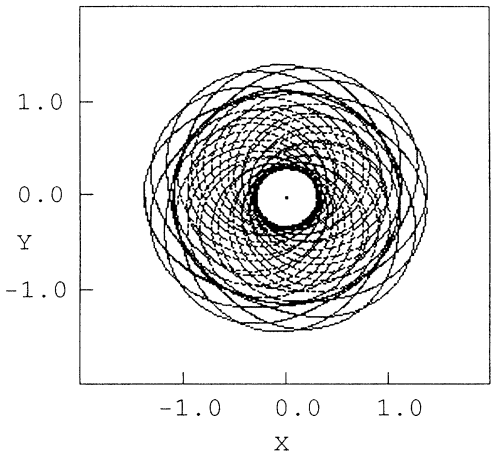

FIG. 2. Braiding torus. Orbits of two electrons are shown for $0 \le t \le 68.4$, using type-1 configuration with $(r_1,v_1)=(1.40,0.86)$.

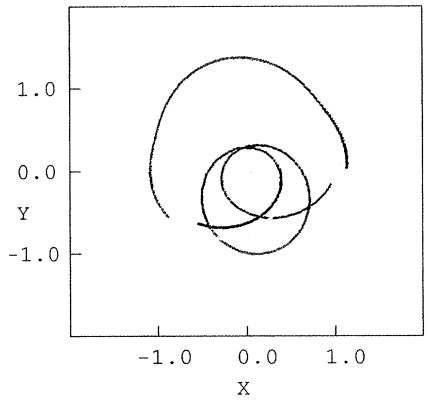

FIG. 3. Orbits of brading torus with color changes every 1.6 time units, from blue to yellow, start from the same initial condition as Fig. 2.

We have adopted the resolution 0.001 for v_1, while r_1 is scanned with the resolution 0.1 for most cases, and with a finer resolution 0.01 near the region where tori are found. If we choose a higher initial value for v_1 than 1.6, one electron is easily ionized, since the electron 1 has a very high energy in the initial state.

For configuration 2, we have checked the initial conditions within $r_1 \in [1.5,3.0]$, $v_1 \in [0.4,1.0]$. Here the resolution for the increment of v_1 is again 0.001, while r_1 is scanned with the resolution 0.5. Within these initial conditions, tori have been found only for $r_1=2.50$ (semicircular case and double ring) and for $r_1=3.00$ (double ring). For larger r_1, trivial double ring tori always exist, since the distance of two electrons is far, and a KAM torus is stable. No nontrivial tori are found in configurations 1 and 2, besides those reported here.

For configuration 3, the search is not systematic. We

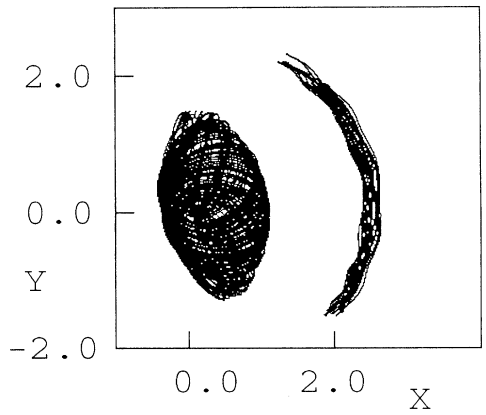

FIG. 4. Semicircular torus with 6:1 locking. Orbits of two electrons are shown for $0 \le t \le 337.6$, using the type-2 initial configuration with $(r_1,v_1)=(2.50,0.40)$.

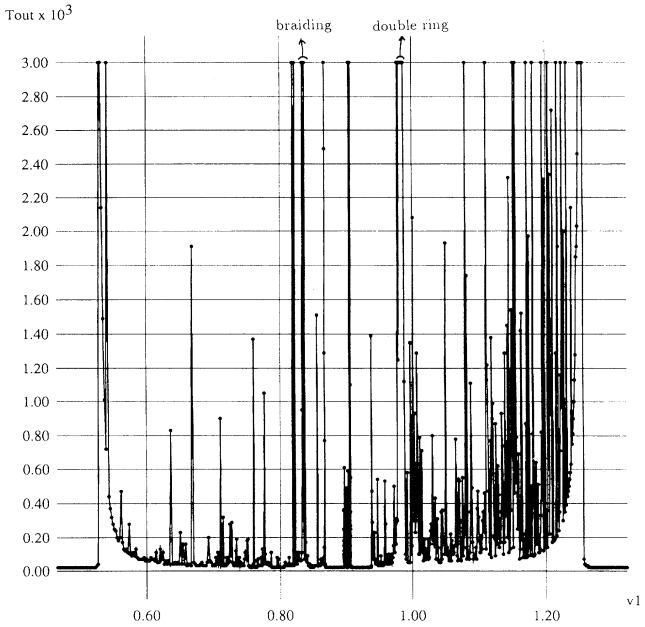

FIG. 5. Ionization time plotted as a function of initial velocity v_1, using the type-1 configuration with $r_1=1.45$. As is shown in the figure, two types of tori exist in separate regions. Cutoff time is chosen to be 3000.

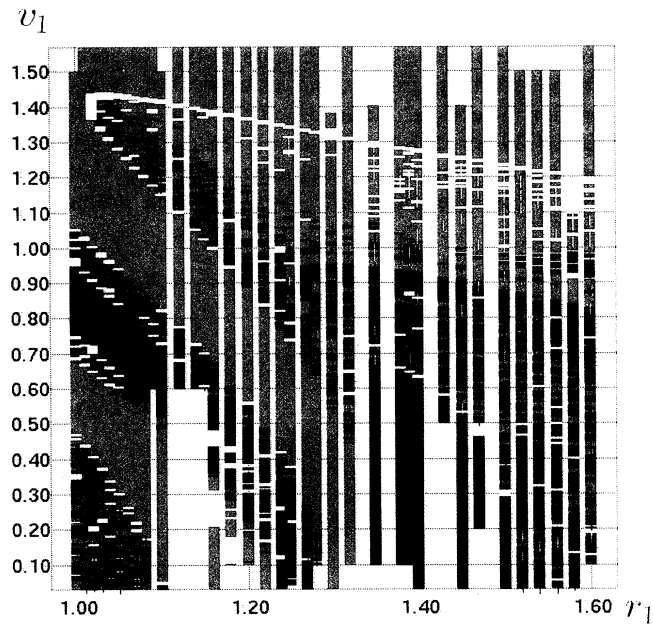

FIG. 6. Initial condition dependence of final state for the type-1 configuration. Color shows the final state: torus (red), ionization of electron 1 (green), ionization of electron 2 (blue), and an orbit close to parabolic one (yellow). The red region around $(r_1,v_1)=(1.50,0.98)$ corresponds to the type A tori, while the type B tori exist in regions too small to be recognized in the figure, around $(r_1,v_1)=(1.40,0.86)$.

have calculated only the neighborhood of the semicircular tori reported in the Letter. For this configuration, the torus we have found is disconnected with the Langmuir's periodic orbit. We have also roughly examined other configurations. They include the case with $r_2 < 0$ at configuration 2, and that with nonparallel speeds for two electrons (with the change of the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$). So far we have found no tori (except a trivial double-ring type), although it is hard to disprove the existence of other types of tori.

As mentioned, all chaotic orbits are ionized as far as we have checked. After some chaotic transients, one of the electrons goes away to infinity. Here, we have computed ionization time as a function of radius for the type-1 configuration, by fixing the ratio of distance r_1/r_2, and varying the ratio of initial velocity v_1/v_2. To check the ionization, we have measured each particle's energy (sum of kinetic energy and potential energy). If the energy of one of the electrons is positive over a given time duration T_{chk} (10 time units), the electron is regarded to be ionized. In Fig. 5 the time necessary for ionization is plotted as a function of the velocity v_1. We have checked this ionization condition for 3000 time units. Thus the peaks (or plateaus) at 3000 mean that the electrons are not ionized before the cutoff time. The torus orbits in the previous examples lie in the plateau region, of course. The other peaks in the figure correspond to an orbit close to parabolic ones, where the energy of the escaping electron is zero, implying the divergence of the ionization time.

The structure in the figure is formed by these parabolic orbits. Within each zone, there are smaller zones successively. (In Fig. 5, some of the edge peaks are missing, which is just due to the precision of the scan of the velocity in the figure.) This type of self-similar structure in a Hamiltonian system is studied by Bleher *et al.* [12], in an escape problem by scattering. Indeed, we have plotted which electron is ionized with the change of an initial velocity of an electron in Fig. 6. The figure clearly shows the fractal-like structure as in [12].

To summarize we have discovered novel types of torus motions in the classical helium atom, while all chaotic orbits are autoionized. According to Einstein's semiclassical quantization, we can get an energy spectrum from tori, when they are not isolated, which is the case in our tori. Within the framework of semiclassical quantization, chaotic orbits may be unnecessary, since they are ionized eventually (this is a result from classical dynamics, but we have to assume the classical-quantum correspondence as long as we use the semiclassical approximation). In this respect, the summation over unstable periodic orbits based on Gutzwiller's formula is not relevant here [13]. Since the classical-quantum correspondence is believed to work better in a high-dimensional dynamical system [14], we may conjecture that the torus-based approach is essential to the analysis of atoms other than hydrogen. In this approach, the interaction among electrons is fully taken into account. The importance of tori rather than chaos will be a common feature here. Discovery of new types of tori with strong interaction between electrons may also provide a new tool for the analysis of strongly correlated electron systems, where the present condensed-matter theory faces with some difficulty [15].

It is an interesting question to search for quantal states corresponding to our tori experimentally (in excited states). The existence of several types of stable tori and parabolic orbits also suggest that there are zones of regions where the ionization is suppressed. The ionization ratio, for example, will take a self-similar structure as in our zone structure, when plotted as a function of input energy.

The authors would like to thank Professor T. Kawai for suggesting this problem to one of us (T.Y.). They would also like to thank Dr. S. Adachi, Dr. T. Konishi, Dr. J. Suzuki, Dr. S. Watanabe, and Dr. M. Matsuzawa for fruitful discussions. This work is partially supported by Grant-in-Aids (No. 04231102) for Scientific Research from the Ministry of Education, Science and Culture of Japan.

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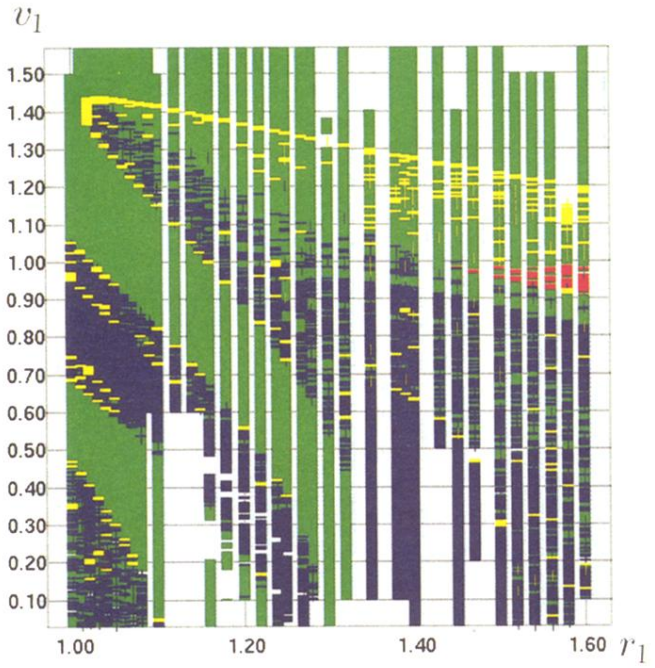
[1] J. H. van Vleck, Philos. Mag. **44**, 842 (1922).
[2] N. Bohr, Philos. Mag. **26**, 492 (1913).
[3] I. Langumuir, Phys. Rev. **17**, 339 (1921).
[4] Von A. Landé, Z. Phys. **2**, 83 (1920).
[5] Albert Einstein, Verch. Dtch. Phys. Ges. **19**, No. 82 (1917).
[6] D. W. Noid and R. A. Marcus, J. Chem. Phys. **67**, 559 (1977).
[7] Martin C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer-Verlag, Berlin, 1990).
[8] While other configurations are roughly surveyed, we have not discovered any other novel tori so far.
[9] This configuration is given from the form 1 with $v_1 < 0$. Here we call the case separately to emphasize the angular momentum dependence.
[10] After the completion of this paper, the authors were informed of the paper by Jörg Müller, Joachim Burgdörfer, and Donald Noid, Phys. Rev. A **45**, 1471 (1992), where semiclassical quantization of this type of torus is studied.
[11] Similar trajectory with other mode locking is noted in K. Richter and D. Wintgen, Phys. Rev. Lett. **65**, 15 (1990).
[12] S. Bleher, C. Greobogi, E. Ott, and R. Brown, Phys. Rev. A **38**, 930 (1988).
[13] G. S. Ezra, K. Richter, G. Tanner, and D. Wintgen, J. Phys. B **24**, L413 (1991). Indeed there are some applications of Gutzwiller's formula to the helium atom by restricting orbits to one-dimensional configuration, where chaotic orbits are stably confined in a finite region.
[14] S. Adachi, M. Toda, and K. Ikeda, Phys. Rev. Lett. **61**, 659 (1988).
[15] Noam Sivan and Shimon Levit, Phys. Rev. B **46**, 2319 (1992).



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