Interaction of the collective and electronic motion of atomic ions in magnetic fields

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In the presence of a homogeneous magnetic field, the center of mass and electronic motion of an atom cannot be separated. For an atomic ion, the residual coupling is a Stark term with an oscillating electric field that is determined by the collective motion of the system. We investigate the effects and phenomena that occur due to this coupling in the classical dynamics of the highly excited ion. In particular, a permanent exchange of energy between the center of mass and the internal degrees of freedom is shown to take place. This leads, in the regular regime, in spite of an initially vanishing center-of-mass velocity, to the *self-stabilization* of the ion on a circular orbit. For small center-of-mass velocities and energies close to the ionization threshold, the motion of the atom is governed by its intermittent behavior. The most interesting dynamics occurs for rapidly moving ions for which the energy transfer from the center of mass to the internal degrees of freedom becomes strong enough to allow the atom to ionize. The statistics of this dynamical *self-ionization* process is studied for different center-of-mass velocities as well as internal energies.

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I. INTRODUCTION

During the past two decades there was an enormous increase of interest in the behavior and properties of matter in strong magnetic fields. The attraction of this field of research certainly also has its origin in the great variety of the observed phenomena. The quantum Hall effect for a two-dimensional extended electron system and the interplay of regularity and chaos for highly excited Rydberg atoms in strong magnetic fields are two exemplary situations from different areas of physics in which the external field plays an outstanding role. In order to observe the above-addressed phenomena it is necessary to achieve magnetic interaction energies that are comparable to or even larger than the relevant Coulomb energies. For an isolated atom at laboratory field strengths this means that we have to consider highly excited states for which the magnetic interaction no longer provides a small perturbation with respect to the electronic structure of the considered system. The paradigm of such an atomic system is the hydrogen atom in a strong magnetic field, whose properties have been investigated in great detail up to and even beyond the field-free ionization threshold (see Ref. [1] and references therein).

In field-free space isolated (Coulomb-)interacting particle systems are invariant with respect to translations in space, i.e., the total canonical momentum is a conserved quantity. In the presence of an external homogeneous magnetic field the space translation symmetry is lost. However, there exists a generalization, the phase-space translation group [2], which provides a symmetry associated with the collective motion of the system. The corresponding conserved quantity is the so-called pseudomomentum [2,3], which is the generalization of the total canonical momentum to the case of the presence of an external magnetic field. The two qualitatively different situations of a neutral and a charged system now have to be distinguished carefully.

For a neutral system the components of the pseudomomentum commute and can be used for a complete pseudoseparaton of the center of mass (c.m.) motion, which eliminates the c.m. coordinates from the Hamiltonian [2–4]. However, this does not mean that the c.m. and the internal motion decouple and indeed the c.m. velocity is, apart from the constant pseudomomentum, completely determined by the components of the internal coordinates perpendicular to the magnetic field. This coupling of the collective and the internal motion has, for highly excited atoms, drastic consequences for the dynamics of both types of motion. Effects due to the inherent two-body character of a neutral two-particle system have been investigated very recently for the hydrogen atom [5–7]. In particular, for the case of a vanishing pseudomomentum it has been observed that the transition from regularity to chaos in the classical internal motion is accompanied by a transition from bounded quasiperiodic oscillations to an unbounded diffusional motion in the c.m. [5]. For a nonvanishing pseudomomentum (or, equivalently, a perpendicular static electric field) and energies close to the ionization threshold the classical dynamics of both the internal as well as the c.m. motion is characterized by its intermittent behavior [6]. For large enough values of the pseudomomentum, an outer potential well is formed, supporting strongly delocalized bound states, which have been studied in detail [7–9].

The subject of investigation of the present paper is the classical interaction of the collective, i.e., c.m., and the

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internal motion for atomic ions, in particular of the He^+ ion, in a magnetic field. For the case of a charged-particle system in a magnetic field, the coupling of the c.m. and the internal degrees of freedom is even more intricate than for the case of a neutral system. One therefore expects a rich classical dynamics to be uncovered if one varies the parameters (field strength, energy, etc.) of the underlying system. These questions have briefly been addressed in a very recent paper [10] and some of the most appealing effects have been reported on. In the present paper we provide an elaborate investigation and discussion of the whole variety of phenomena appearing in the classical dynamics of the above system.

The paper is organized as follows. In Sec. II we introduce the Hamiltonian, its constants of motion, and the coupled equations of motion for the c.m. as well as electronic degrees of freedom. In Sec. III we present and discuss the results of our investigation of the c.m. and the electronic motion of the ion. Two major effects can be observed: first, the self-stabilization of the ion on a Landau orbit under regular conditions and for vanishing initial c.m. velocity and, second, the self-ionization process for fast ions by energy transfer from the c.m. to the internal degrees of freedom. Regular, chaotic, and intermittent dynamics are observed and lead to a variety of different possibilities of the behavior of the c.m. and the electronic degrees of freedom. Finally, we discuss in the Appendix our method for the numerical integration of the classical equations of motion of the He^+ ion in a strong magnetic field.

II. THE HAMILTONIAN AND THE EQUATIONS OF MOTION

The general problem we are concerned with is a charged two-body system interacting via the Coulomb potential in the presence of an external, strong, homogeneous magnetic field. As already mentioned in the Introduction, the pseudomomentum $\mathbf{K}$ is a conserved quantity for this system and represents a generalization of the c.m. momentum in field-free space to the situation in the presence of a magnetic field [11]

$$\mathbf{K}=\sum_{i=1}^{2}(\mathbf{p}_i-q_i\mathbf{A}_i+q_i\mathbf{B}\times\mathbf{r}_i)\ , \tag{1}$$

where $\mathbf{r}_i$ and $\mathbf{p}_i$ are the Cartesian coordinates and momenta in the laboratory coordinate system. $\mathbf{A}$ and $\mathbf{B}$ are the vector potential and magnetic field, respectively. In contrast to the case of a neutral system, the two components of the pseudomomentum are, for a charged system, not independent, i.e., they have a nonvanishing commutator that is proportional to the net charge Q of the system [2–4]

$$[\mathbf{K}_\alpha,\mathbf{K}_\beta]=-iQ\epsilon_{\alpha\beta\gamma}\mathbf{B}_\gamma\ , \tag{2}$$

where $\epsilon_{\alpha\beta\gamma}$ is the Levi-Civita tensor. For an ion therefore it is impossible to eliminate the c.m. coordinates completely from the Hamiltonian by introducing the pseudomomentum as a canonical conjugated momentum. This is a major difference from the case of a neutral system for which such an elimination is possible [2–4]. Nevertheless, the transformations introduced for a neutral system to perform the so-called pseudoseparation of the c.m. motion can, in a modified version, be also applied to the case of a charged-particle system [3,4,12]. The resulting transformed Hamiltonian takes on a particularly appealing form and reads, for the He^+ ion, as

$$\mathcal{H}=\mathcal{H}_1+\mathcal{H}_2+\mathcal{H}_3\ , \tag{3}$$

where

$$\mathcal{H}_1=\frac{1}{2M}\left[\mathbf{P}-\frac{Q}{2}\mathbf{B}\times\mathbf{R}\right]^2\ , \tag{3a}$$

$$\mathcal{H}_2=e\frac{\alpha}{M}\left[\mathbf{B}\times\left[\mathbf{P}-\frac{Q}{2}\mathbf{B}\times\mathbf{R}\right]\right]\mathbf{r}\ , \tag{3b}$$

$$\mathcal{H}_3=\frac{1}{2m}\left[\mathbf{p}-\frac{e}{2}\mathbf{B}\times\mathbf{r}+\frac{Q}{2}\frac{m^2}{M^2}\mathbf{B}\times\mathbf{r}\right]^2 +\frac{1}{2M_0}\left[\mathbf{p}+\left[\frac{e}{2}-\frac{Q}{2M}\frac{m}{M}(M+M_0)\right]\mathbf{B}\times\mathbf{r}\right]^2+V\ , \tag{3c}$$

where m, M_0, and M are the electron, the nuclear, and the total mass, respectively. $\alpha=(M_0+Zm)/M$ and V is the Coulomb potential. The magnetic-field vector $\mathbf{B}$ is, in the following, assumed to point along the z axis. $(\mathbf{R},\mathbf{P})$ and $(\mathbf{r},\mathbf{p})$ are the canonical pairs of variables for the c.m. and the relative motion, respectively. The Hamiltonian $\mathcal{H}$ involves five degrees of freedom since the center-of-mass motion parallel to the magnetic field is a free translational motion, i.e., separated completely. According to Eq. (2), the parallel and the perpendicular components of the pseudomomentum commute and it is therefore in principle possible to eliminate also one of the two perpendicular components of the c.m. coordinate vector. However, this would not yield any further simplification of the Newtonian equations of motion, which will be solved below and for which we will explicitly use the conservation of the pseudomomentum [see Eqs. (6) and (A7)].

The Hamiltonian $\mathcal{H}$ consists of three parts that correspond to different types of motion or interaction. The part $\mathcal{H}_1$ in Eq. (3a), which involves solely the c.m. degrees of freedom, describes the cyclotron motion of a free pseudoparticle with mass M and charge Q in a homogeneous magnetic field. Within the Hamiltonian $\mathcal{H}_1$ the ion is therefore treated as an entity with the net charge and the total mass of the ion. This can be looked at as a zeroth-order approximation to the real c.m. motion. We will see in Sec. III that this zeroth-order picture is, in general, not sufficient to describe the c.m. motion of the ion. In fact, the behavior of the c.m. can deviate strongly from the motion given by the Hamiltonian $\mathcal{H}_1$ and exhibits a variety of different phenomena depending on the parameter values (energy, field strength, c.m. velocity). The origin of this rich dynamics lies in particular in the Hamiltonian $\mathcal{H}_2$ in Eq. (3b), which describes the coupling of the c.m. and the electronic degrees of freedom. The Hamil-

tonian $\mathcal{H}_2$ represents a motional Stark term with a rapidly oscillating electric field, which is determined by the dynamics of the system. Because of this "dynamical" electric field the collective and the internal motion will, in general, mix up heavily. Finally, $\mathcal{H}_3$ in Eq. (3c) contains only the electronic degrees of freedom and describes, to zeroth order, the relative motion of the electron with respect to the nucleus.

An alternative way of writing the Hamiltonian $\mathcal{H}$ is

$$\mathcal{H}=\frac{1}{2M}\left[\mathbf{P}-\frac{Q}{2}\mathbf{B}\times\mathbf{R}-e\alpha\mathbf{B}\times\mathbf{r}\right]^2 + \frac{1}{2\mu}\left[\mathbf{p}-\frac{e}{2M^2}(M_0^2-Zm^2)\mathbf{B}\times\mathbf{r}\right]^2+V\ , \quad (4)$$

where $\mu=mM_0/M$ is the reduced mass. This reformulation of the Hamiltonian as a sum of two quadratic terms plus the Coulomb potential gives us some additional insight into the problem. The two Hamiltonian equations of motion

$$\dot{\mathbf{R}}=\frac{1}{M}\left[\mathbf{P}-\frac{Q}{2}\mathbf{B}\times\mathbf{R}-e\alpha\mathbf{B}\times\mathbf{r}\right]\ , \quad (4a)$$

$$\dot{\mathbf{r}}=\frac{1}{\mu}\left[\mathbf{p}-\frac{e}{2M^2}(M_0^2-Zm^2)\mathbf{B}\times\mathbf{r}\right] \quad (4b)$$

belonging to $\mathcal{H}$ immediately allow us to identify the first quadratic term in Eq. (4) as the kinetic energy $E_{\text{c.m.}}=(M/2)\dot{\mathbf{R}}^2$ of the c.m., whereas the second quadratic term represents the kinetic energy of the electronic relative motion $(\mu/2)\dot{\mathbf{r}}^2$. The kinetic energy of the c.m. therefore depends on the electronic degrees of freedom.

For our understanding and interpretation of the dynamics of the ion later on it is also instructive to examine the Newtonian equations of motion. They take on the forms

$$M\ddot{\mathbf{R}}+Q\mathbf{B}\times\dot{\mathbf{R}}+e\alpha\mathbf{B}\times\dot{\mathbf{r}}=0\ , \quad (5a)$$

$$\mu\ddot{\mathbf{r}}+\frac{e}{M^2}(M_0^2-Zm^2)\mathbf{B}\times\dot{\mathbf{r}}+e\alpha\mathbf{B}\times\dot{\mathbf{R}}+\frac{\partial V}{\partial\mathbf{r}}=0\ . \quad (5b)$$

Again the mutual dependence of the c.m. and the electronic degrees of freedom becomes obvious. Equation (5a) can be integrated once and yields an integration constant that is the pseudomomentum in terms of the c.m. velocity and the c.m. and the electronic coordinates

$$\mathbf{K}=M\dot{\mathbf{R}}+Q\mathbf{B}\times\mathbf{R}+e\alpha\mathbf{B}\times\mathbf{r}\ . \quad (6)$$

Next let us establish the equations of motion for the c.m. energy $E_{\text{c.m.}}$ and for the internal energy, which is defined as $E_{\text{int}}=(\mu/2)\dot{\mathbf{r}}^2+V$. Multiplying Eq. (5a) with the c.m. velocity we obtain the following expression for the time derivative of the c.m. and the internal energy

$$\frac{d}{dt}E_{\text{c.m.}}=-\frac{d}{dt}E_{\text{int}}=e\alpha(\mathbf{B}\times\dot{\mathbf{R}})\dot{\mathbf{r}}\ . \quad (7)$$

This equation shows that a permanent flow of energy from the c.m. to the electronic degrees of freedom and vice versa has to be expected. In Sec. III Eq. (7) will be most helpful for our understanding of the mechanism of the energy transfer between the collective and the electronic motion.

III. RESULTS AND DISCUSSION

In this section we elaborate and discuss the results of our comprehensive study of the classical dynamics of the He^+ ion. We thereby have to solve the corresponding Newtonian equations of motion (5a) and (5b) that contain five coupled degrees of freedom. This is a nontrivial task since the long integration times necessary to observe the different time scales occurring in the dynamics of the ion (see below) require not only a fast integration algorithm but also a very high accuracy and therefore large step size. To achieve these goals we have to smoothen and regularize the Newtonian equations of motion (5a) and (5b) and in particular we have to get rid of the singularity due to the Coulomb potential term. Both our transformations of the equations of motion as well as the numerical integration algorithm will be discussed in the Appendix. It is important to note that without these techniques the present investigation would not have been possible.

A. The self-stabilization effect in the regular regime

Let us begin our investigation of the classical dynamics of the He^+ ion with the regime for which the complete phase space is regular. The internal energy E_{int} and the field strength are chosen such that the Coulomb potential dominates over the magnetic interaction terms. In addition, we first of all focus on the case of vanishing initial c.m. velocity, i.e., $V_{\text{c.m.}}=|\dot{\mathbf{R}}|=0$. In the absence of a magnetic field there is no coupling between the c.m. and the electronic degrees of freedom and for the special case $V_{\text{c.m.}}=0$ the c.m. of the ion simply is at rest. Figures 1(a)–1(g) show the behavior of a typical c.m. trajectory in the presence of magnetic field for different time periods. Since the Coulomb interaction dominates over the magnetic energies, the shortest time scale T_1, which is approximately 4×10^3 a.u. for the parameter values of Fig. 1, is given by one perturbed Kepler cycle in the internal motion. Figure 1(a) shows the five oscillations of the c.m. motion in the $(X_{\text{c.m.}},Y_{\text{c.m.}})$-coordinate plane perpendicular to the magnetic field, which correspond to five Kepler cycles in the internal motion. Figure 1(b) shows the time dependence of the c.m. kinetic energy for the same time period. First of all we observe that the initially vanishing c.m. kinetic energy increases to some maximal value and subsequently decreases and so on, i.e., it oscillates. The origin of this oscillating flow of energy between the c.m. and the internal degrees of freedom is the coupling term $\mathcal{H}_2$ in Eqs. (3) and (3b). The rate of energy exchange between the internal and the c.m. degrees of freedom is governed by formula (7). This equation tells us that extrema in the c.m. and internal energies do occur for configurations for which the projections of the c.m. and the electronic velocity vectors onto the plane perpendicular to the magnetic field are parallel, i.e., $\dot{\mathbf{R}}_\perp\|\dot{\mathbf{r}}_\perp$. A strong exchange of energy has to be expected for the opposite case for which the projections of the two velocity vectors

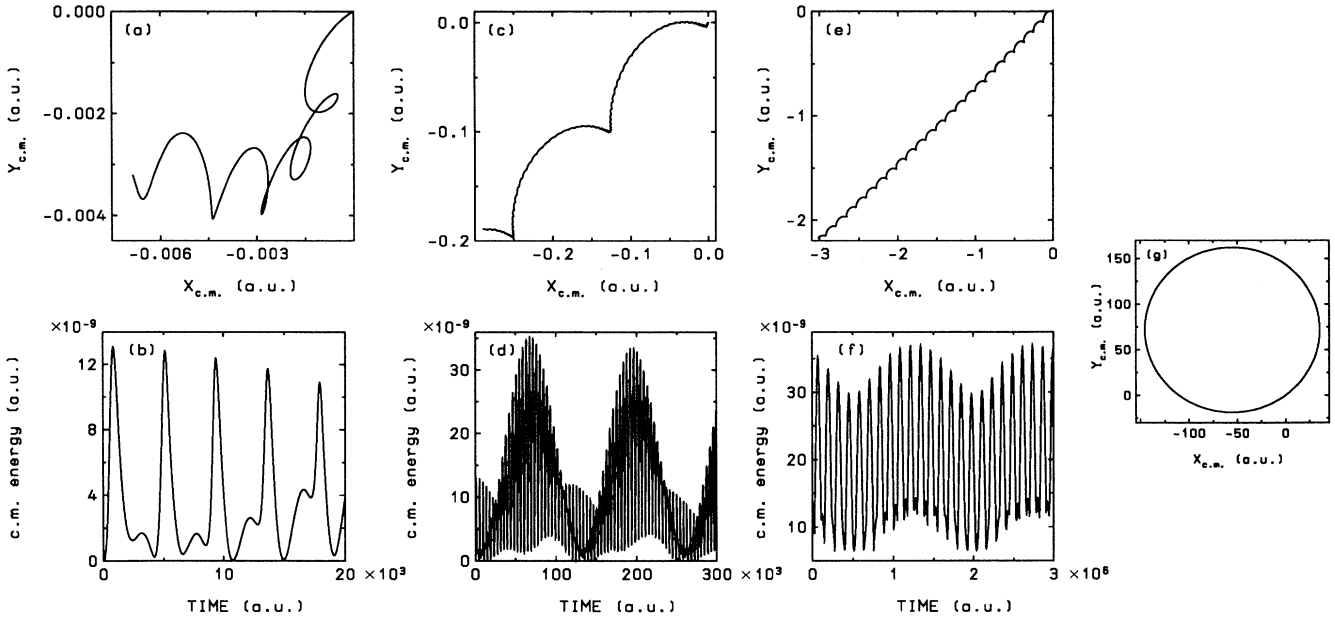

FIG. 1. (a), (c), (e), and (g) show the c.m. motion in the coordinate plane perpendicular to the magnetic field for the same trajectory with increasing propagation times 2×10^4, 3×10^5, 3×10^6, and 5×10^8 a.u., respectively. (b), (d), and (f) show correspondingly the time dependence of the c.m. energy for the same trajectory. The initial c.m. velocity is equal to zero. The parameter values are $E_{\rm int}=-10^{-2}$ a.u. and $B=10^{-4}$ a.u. All values are given in atomic units.

are perpendicular to each other, i.e., $\dot{\mathbf{R}}_\perp \perp \dot{\mathbf{r}}_\perp$.

Next we consider Figs. 1(c) and 1(d), which illustrate the same c.m. trajectory as in Figs. 1(a) and 1(b), respectively, but for a time period that is about 15 times longer. We immediately realize that the amplitudes of the individual oscillations of the c.m. energy are periodically modulated on a characteristic time scale $T_2\approx 30T_1$. The corresponding motion of the c.m. in the plane perpendicular to the magnetic field shows an additional oscillatory behavior of period T_2. This second time scale T_2 arises due to the fact that the magnetic field causes, via the electronic Zeeman term $-(e/2)[(M_0^2-Zm^2)/mMM_0]\mathbf{B}(\mathbf{r}\times\mathbf{p})$ [see $\mathcal{H}_3$ in Eq. (3c)], a rotation of the Kepler ellipses of the internal motion. T_2 is therefore approximately the time period of a complete rotation of these ellipses.

If we consider the motion of the c.m. and the time dependence of its energy on an even larger time scale T_3, which is about ten times T_2, we arrive at the behavior illustrated in Figs. 1(e) and 1(f), respectively. Figure 1(e) shows, for the c.m. motion in the $(X_{\rm c.m.},Y_{\rm c.m.})$-coordinate plane, a straight uniform motion on the time scale T_3, which possesses periodic modulations of small amplitudes on the two shorter time scales T_2 and T_1. [The individual oscillations on the time scale T_1 according to Fig. 1(a) are not visible in Fig. 1(e).] Figure 1(f) shows us the corresponding time dependence not directly of the c.m. kinetic energy but of the maxima of the c.m. energy. We observe on top of the oscillations of the maxima another periodic modulation of the amplitudes of the "maxima oscillations" on the time scale T_3. The time period T_3 is associated with a period of changes of the orbital parameters of the ellipses in the internal motion, which arises due to the diamagnetic electronic term in the Hamiltonian $\mathcal{H}_3$ [13] [see Eqs. (3) and (3c)]. The occurrence of all the time scales T_1, T_2, T_3 and, as we shall see below, also T_4 in the c.m. motion is, of course, due to the action of the coupling Hamiltonian $\mathcal{H}_2$.

Finally, we have illustrated in Fig. 1(g) the c.m. motion for a time period $T_4=5\times10^8$ a.u., which is two orders of magnitude larger than the time scale T_3. The locally straight uniform motion shown in Fig. 1(e) closes to a circular orbit on a coordinate range of a few hundred atomic units. The oscillatory motions of the c.m. belonging to the shorter-time scales T_1, T_2, and T_3 take place on a coordinate range of typically a few 10^{-3}, 10^{-1}, and 10^0 a.u., respectively, and are therefore not observable in Fig. 1(g). The circular orbit of Fig. 1(g) corresponds to the long-time behavior of the c.m. and might bring us to the idea that the c.m. motion on the long-time scale could be that of a free pseudoparticle with charge Q and mass M in a homogeneous magnetic field. However, we have chosen as an initial condition a vanishing c.m. velocity and therefore it is by no means evident what the radius and the angular frequency of the long-time circular motion should be. The observed effect of the *self-stabilization of the ion* with vanishing initial c.m. velocity on a circular (cyclotron) orbit has its origin in the subtle interaction of the c.m. and electronic degrees of freedom. In order to understand this effect in a more quantitative way and to derive explicit expressions for the radius and the angular frequency of the circular c.m. motion on a long-time period, we must have a closer look at the Newtonian equations of motion (5a) and (5b) and the ex-

pression for the pseudomomentum $\mathbf{K}$ in Eq. (6).

For a free particle with charge Q in a homogeneous magnetic field the expression $-(1/QB^2)(\mathbf{B}\times\mathbf{K})$ gives us the position vector of the midpoint of the cyclotron orbit [2–4]. Considering the ion as a pseudoparticle we can therefore reformulate Eq. (6) as a differential equation for the radius vector

$$\mathbf{R}_c=\mathbf{R}+\frac{1}{QB^2}(\mathbf{B}\times\mathbf{K}) \tag{8}$$

and, using the fact that the pseudomomentum is a conserved quantity, we arrive at

$$M\dot{\mathbf{R}}_c+Q\mathbf{B}\times\mathbf{R}_c+e\alpha\mathbf{B}\times\mathbf{r}=\mathbf{0}\ . \tag{9}$$

As a next step we project onto the azimuthal c.m. velocity component V_t in order to obtain the angular frequency, i.e., we multiply Eq. (9) by the unit vector perpendicular to the radius vector $\mathbf{R}_c$, i.e., by $(\mathbf{R}_c\times\mathbf{B})/BR_c$. With a little algebra this yields

$$V_t=\frac{B}{MR_c}[QR_c^2+e\alpha(\mathbf{r}\mathbf{R}_c)]\ . \tag{10}$$

Now, since we are interested in the averaged behavior on the time scale T_4, we calculate the mean of Eq. (10) by integrating over a typical time period $T_4\gg T>T_3$. Since we refer to the pseudoparticle picture R_c is approximately constant and in particular the time average of the second term in Eq. (10) is negligible. (Remember that $\mathbf{r}$ is oscillating with period $T_1\ll T$.) We therefore obtain the mean azimuthal velocity $\bar{V}_t$ and consequently the angular frequency Ω_c to

$$\bar{V}_t=\frac{QBR_c}{M},\quad \Omega_c=\frac{QB}{M}\ . \tag{11}$$

The radius R_c of the circular c.m. motion can be expressed in terms of the initial conditions of the considered trajectory. To achieve this we insert in Eq. (8) the expression for the pseudomomentum in Eq. (6) at $t=0$. The resulting equation for the radius R_c takes on the form

$$R_c=\left|\frac{M}{QB^2}\mathbf{B}\times\dot{\mathbf{R}}-\alpha\frac{e}{Q}\mathbf{r}_\perp\right|_{(t=0)}\ . \tag{12}$$

For our special case of vanishing initial c.m. velocity $\dot{\mathbf{R}}(0)=\mathbf{0}$ this means that the radius of the effectively circular orbit of the c.m. on the long-time scale is completely determined by the component perpendicular to the magnetic field of the initial distance of the electron from the nucleus, i.e., $R_c=-\alpha(e/Q)|\mathbf{r}_\perp(0)|$. This is an amazing result, which again is a consequence of the action of the coupling terms between the c.m. and the internal electronic motion. In particular, we can obtain any radius R_c belonging to the allowed range of values of $\mathbf{r}_\perp(0)$ by choosing the appropriate initial values for the electronic coordinate $\mathbf{r}_\perp$.

Addition valuable information concerning the long-time circular motion of the c.m. of the ion is the mean value of the c.m. energy $\bar{E}_{\text{c.m.}}$. The latter quantity has to be carefully distinguished from the kinetic energy belonging to the mean azimuthal velocity since the squared average of $\dot{\mathbf{R}}$ differs from the average of the square $\dot{\mathbf{R}}^2$ (see below). Starting with the definition

$$\bar{E}_{\text{c.m.}}=\frac{1}{T}\int_0^T\frac{M}{2}\dot{\mathbf{R}}^2dt \tag{13}$$

for some typical integration time $T_4\gg T>T_3$ and using the expression for the pseudomomentum in Eq. (6) as well as Eq. (8) and the fact that the time average of the scalar product $(\mathbf{r}\mathbf{R}_c)$ is negligible, we arrive at the following expression for the mean energy of the c.m.:

$$\bar{E}_{\text{c.m.}}=\frac{B^2}{2M}(Q^2R_c^2+e^2\alpha^2\Upsilon^2)\ , \tag{14}$$

where

$$\Upsilon^2=\frac{1}{T}\int_0^T\mathbf{r}_\perp^2dt \tag{15}$$

is the mean of the square of the perpendicular component of the electronic coordinate vector. The first term in Eq. (14) is the mean energy of the c.m. due to its azimuthal motion $(M/2)\bar{V}_t^2$, whereas the second term is due to the radial kinetic energy that belongs to the motion on the time scales T_1, T_2, and T_3. Comparing the above analytical results for the angular frequency, the radius, and the mean energy with the corresponding numerical values yields excellent agreement. In addition, it is possible to derive an expression for the mean c.m. velocity, which, however, is more complicated and also less instructive than the above presented quantities. To conclude our discussion of the case $|\dot{\mathbf{R}}(0)|=\mathbf{0}$ let us mention that the occurrence of the above-discussed four, by different orders of magnitude, time scales in the motion of the ion is characteristic for parameter values (energies, field strength) that correspond to the deep regular regime. With, for example, increasing internal energy the time scales $\{T_i\}$ can become comparable and the above-discussed separation into individual oscillations and modulations is then no longer possible.

Let us now briefly consider the case of finite, but not too large, c.m. velocity. With increasing initial c.m. velocity the first term on the right-hand side of Eq. (12) becomes more and more important and finally dominates over the second term, which depends only on the electronic coordinates. In this case the mean c.m. energy is also dominated by the first term in Eq. (14). The amplitude of the oscillations of the c.m. energy divided by the corresponding mean value becomes smaller with increasing initial c.m. velocity and correspondingly the amplitude of the oscillations of the c.m. motion in coordinate space belonging to the time scales T_1, T_2, and T_3 divided by the mean traveled distance of the c.m. also becomes smaller. From first glance it might then seem that the ion could be approximately treated as a free pseudoparticle without any coupling of the c.m. to the electronic degrees of freedom. However, as we shall see in Sec. III D, also in this case the coupling of the c.m. and the electronic degrees of freedom has drastic consequences for the dynamical behavior of the ion.

B. The chaotic regime

In the present subsection we consider the case of chaotic dynamics for the internal as well as the c.m. motion. The parameter values, i.e., the magnetic field strength, the initial internal energy, and the internal angular momentum, are chosen such that the Coulomb interaction and the magnetic energies are of comparable order of magnitude. These parameter values would yield a completely chaotic phase space for the case of the He^+ ion with the assumption of an infinite nuclear mass. Furthermore, we restrict our discussion to the case of vanishing initial c.m. velocity. The effects and the dynamics for finite c.m. velocity will be discussed in detail in Secs. III C and III D.

In Figs. 2(a) and 2(b) we show, for a typical trajectory, the motion of the c.m. in the plane perpendicular to the magnetic field for two different time periods. For the shorter time period $T=10^7$ a.u. of Fig. 2(a), the c.m. motion looks like a randomlike unbounded motion, which exhibits none of the regular structure or different time scales of motion discussed in Sec. III A. The question therefore arises to what extent the long-time circular motion of the c.m., observed in the regular regime, survives in the chaotic regime. To give an answer to this question we illustrate in Fig. 2(b) the behavior of the c.m.

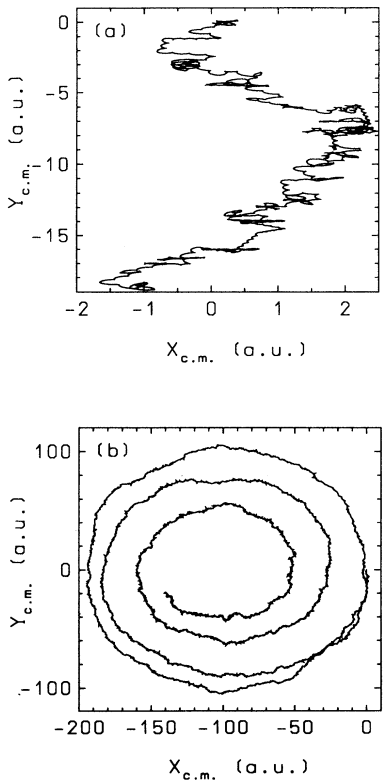

FIG. 2. c.m. motion in the coordinate plane perpendicular to the magnetic field for a chaotic trajectory: (a) for the time interval 10^7 a.u. and (b) for the time interval 1.6×10^9 a.u. The initial c.m. velocity is equal to zero. The parameter values are $E_{\rm int}=-3.4\times10^{-4}$ a.u. and $B=10^{-4}$ a.u. All values are given in atomic units.

for a time period $T=1.6\times10^9$ a.u. Also on the long-time scale we observe severe deviations of the c.m. motion from the circular motion observed in the regular regime: the circular shape is strongly disturbed even within one cycle and the c.m. leaves the suspected circular orbit completely within a few cycles. The radius we would have expected according to Eq. (12) if the initial conditions would have been regular is $R_c\approx100$ a.u.

In the following two subsections we will investigate the dynamical effects of the interaction of the c.m. and the electronic degrees of freedom with increasing c.m. velocity ending up with the case of a rapidly moving He^+ ion in a magnetic field.

C. Intermittency: A characteristic near-threshold phenomenon

In the present subsection we study the dynamics of the c.m. as well as electronic motion of the ion for total energies that are slightly greater than zero. The internal energies are chosen such that the corresponding He^+ ion with the assumption of an infinite nuclear mass shows a completely chaotic phase space. For a strong laboratory field strength of $B=10^{-4}$ a.u., i.e., 23.5 T, this means that the internal energies are in the range $-3.4\times10^{-4}\le E_{\rm int}<0$ a.u., whereas the total energies are of the order of magnitude $10^{-3}\ge E>0$ a.u., which corresponds to c.m. velocities less than 5×10^{-4} a.u., i.e, 1.1×10^3 m s^{-1}.

As a characteristic phenomenon in the above range of energies and/or field strengths we observe the intermittent behavior of the c.m. as well as electronic motion. Figures 3(a)–3(e) illustrate the behavior of the different c.m. and electronic quantities for a typical intermittent trajectory. Let us begin our discussion with the time dependence of the c.m. energy, which is shown in Fig. 3(a). After an initial phase of irregular oscillations there occurs a sudden drop at approximately $T=2.5\times10^8$ a.u. and the c.m. energy decreases to about half of its initial value. After oscillating back at approximately $T=5\times10^8$ a.u. another phase of irregular oscillations follows and so on. The bursts of large energy loss in the c.m. occur at irregular intervals and are, according to Fig. 3(b), accompanied by a sudden increase of the internal energy. This is of course a consequence of the conservation of the total energy. For our chosen example the internal energy remains also during the bursts of strong energy flow below the escape, i.e, zero energy threshold. The dynamical behavior of the c.m. and the internal energies, shown in Figs. 3(a) and 3(b), respectively, is governed by the equations of motion (7) and the variety of their solutions reflects the different possibilities in the behavior of the c.m. and electronic velocities.

What happens to the electronic and the c.m. motion during these alternating phases of irregular energy oscillations and bursts of energy transfer? Figure 3(c) shows the internal electronic motion in the coordinate plane perpendicular to the magnetic field. There exist two alternating phases of motion. During one phase the electron and the nucleus are close together and interact strongly, i.e., the Coulomb and the magnetic energies are

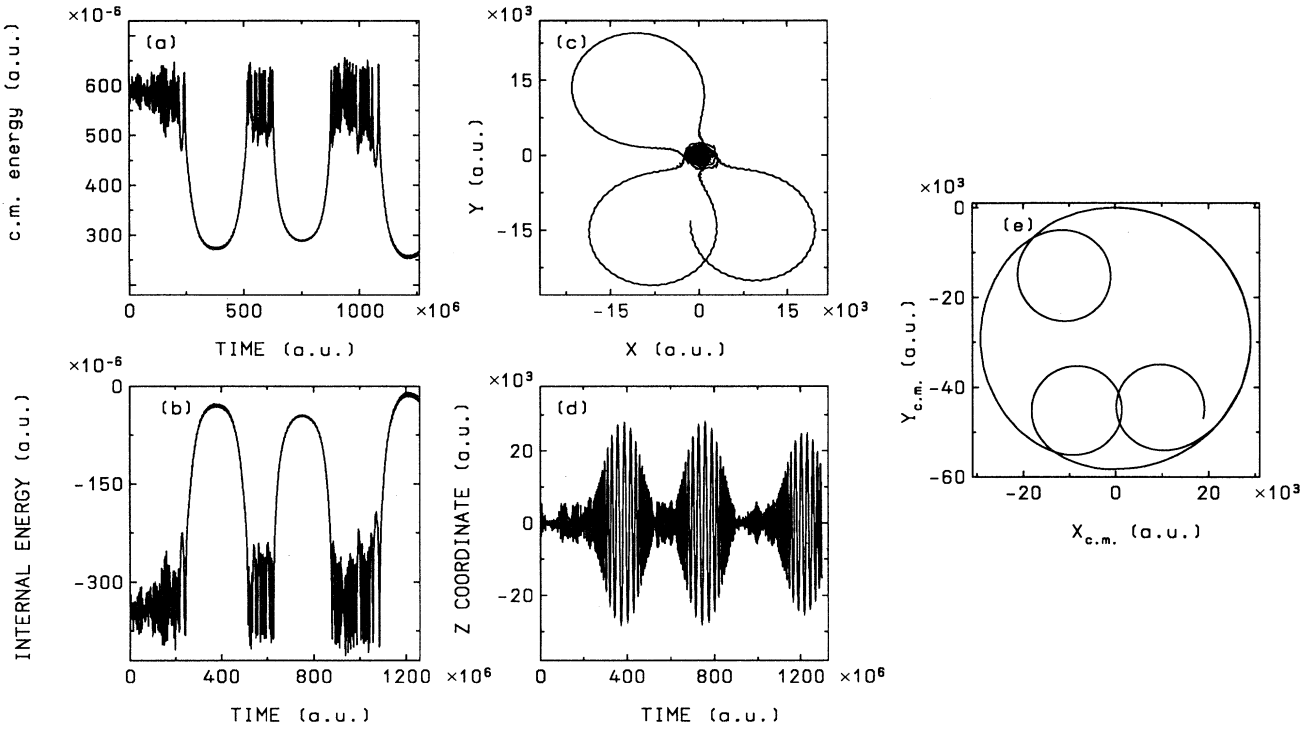

FIG. 3. c.m. and electronic motion of an intermittent trajectory for a propagation time of 1.3×10^{9} a.u. (a) and (b) show the time dependence of the c.m. and the internal energy, respectively. (c) illustrates the relative motion in the coordinate plane perpendicular to the magnetic field. (d) shows the corresponding time dependence of the component of the relative coordinate parallel to the magnetic field. (e) illustrates the c.m. motion in the plane perpendicular to the magnetic field. The parameter values are $E_{\rm int}=-3.4\times10^{-4}$ a.u. and $B=10^{-4}$ a.u. and the initial c.m. velocity is 4×10^{-4} a.u. All values are given in atomic units.

of comparable order of magnitude. These periods of motion correspond to the black bubble in Fig. 3(c). Within the concept of the determination of local Ljapunov exponents [14,15] this means that we obtain a nonvanishing local Ljapunov exponent and therefore we will refer to this phase as a chaotic one. It corresponds to the periods of irregular oscillations in the c.m. as well as the internal energies, shown in Figs. 3(a) and 3(b), respectively. The second phase of the electronic motion plotted in Fig. 3(c) is a large-amplitude (note the large coordinate range) quasiregular motion of circular shape that has a vanishing local Ljapunov exponent. During this period of motion the magnetic forces dominate over the Coulomb interaction, which provides only a small perturbation. The quasiregular phases of motion correspond to the situation of strongly increased internal and therefore lowered c.m. energies, which occur, in Fig. 3(a), for example, in the time interval $2.5\times10^{8}<T<5\times10^{8}$ a.u.

In Fig. 3(d) the z component of the internal coordinate is illustrated as a function of time. The chaotic phase of motion corresponds to the irregular oscillations of small amplitude, whereas the quasiregular phase consists of large-amplitude oscillations in the z coordinate. The circularlike motion in the plane perpendicular to the magnetic field [see Fig. 3(c)] is therefore accompanied by huge oscillations in the direction parallel to the field. An analysis of the motion illustrated in Fig. 3(b) by considering its power spectrum clearly shows a $1/f^{\mu}$ scaling behavior over many decades, which is due to the chaotic part of the motion, and on top of it at small values of the frequency a broad peak, which arises due to the quasiregular phase of large amplitude oscillations. The striking feature of the trajectories is therefore their intermittent behavior that consists of alternating phases of chaotic and quasiregular motion. The latter phase is initiated by a rapid energy transfer process from the c.m. to the internal motion. We emphasize that intermittency is, for the parameter values considered in the present subsection, a generic phenomenon in phase space.

Let us now consider how the intermittent behavior shows up in the c.m. motion of the atom. To this purpose we have illustrated in Fig. 3(e) the c.m. motion in the coordinate plane perpendicular to the magnetic field. We observe an approximately circular motion with a radius of about 3×10^{4} a.u., which contains circles of smaller radius. The small circles correspond to the quasiperiodic phases of motion during which the system is very weakly bound and the c.m. motion is approximately given by the motion of the bare helium nucleus with charge $-2e$ in a magnetic field. The large circle corresponds to the chaotic phase of motion during which the system is strongly bound. However, the chaoticity is "too weak" in order to be "observed" on the time scale of Fig. 3(e). The radius of the large circle is therefore approximately given by Eq. (12), which is based on the picture of the motion of a pseudoparticle with charge Q and

mass M in a magnetic field and has been discussed in detail in Sec. III A. The intermittent behavior in the electronic motion therefore reflects itself in the c.m. motion by alternating phases of almost circular motions with different radii. Finally, we mention that intermittency has also been observed and investigated for the highly excited hydrogen atom with a large pseudomomentum. Although the manifestation of intermittency is for the present case of an ion quite different from that of the neutral hydrogen atom, the mechanisms are very similar. Concerning the details of this mechanism we therefore refer the reader to the literature [6].

D. The self-ionization process for fast atomic ions

In the context of the discussion of the intermittent dynamics of the ion we observed in the preceding subsection that, after a period of oscillations in the c.m. energy, there occurs a strong flow of energy from the c.m. to the electronic degrees of freedom [cf. Fig. 3(a)]. This sudden decrease in the c.m. energy introduces the quasiregular phase of a weakly bound electronic motion. The natural question now arises whether the energy transfer can become large enough in order to ionize the atom. To investigate this we consider in the present subsection fast He^+ ions, i.e., we study the classical dynamics of the ion for large initial c.m. velocities.

Let us first consider parameter values, i.e., initial internal energies and field strengths, for which the corresponding phase space of the He^+ ion with the assumption of an infinite nuclear mass is completely regular. The initial internal energies correspond to an electronically highly excited ion. Since the free motion of a charged particle in a homogeneous magnetic field is confined to a certain coordinate range, ionization, i.e., infinite separation of an electron from the remaining charged core of an atom, is, in the presence of a magnetic field, only possible in the direction parallel to the magnetic field. In Figs. 4(a) and 4(b) we illustrate the time dependence of the component of the electronic coordinate parallel to the magnetic field as well as the time dependence of the c.m. energy, respectively, for a typical trajectory. The initial c.m. energy is 12.2677 a.u., which is many orders of magnitude larger than the internal energy but still well within the regime for which a nonrelativistic approach is valid. After a transient time $T=7\times10^6$ a.u. of many bound regular oscillations in the internal motion, a strong flow of energy from the c.m. to the internal motion takes place. The internal energy is hereby increased above the threshold for ionization $E_{\text{int}}=0$ and the ion immediately ionizes, i.e., the electron escapes in the direction parallel to the magnetic field. The transferred energy, which is, in our case of Figs. 4(a) and 4(b), approximately 6×10^{-3} a.u., corresponds to only a small fraction of the total initial c.m. energy. Again it is worth noting that the observed ionization process via energy transfer from the c.m. to the electronic motion is only possible due to the presence of the coupling term $\mathcal{H}_2$ in the Hamiltonian (3).

Next let us consider the ionization process for initial internal energies and field strengths that yield a completely chaotic phase space for the corresponding He^+ ion with the assumption of an infinite nuclear mass. Figures 4(c) and 4(d) again show the electronic coordinate component parallel to the field and the c.m. energy, respectively, as a function of time for a typical trajectory. Starting with an initial c.m. energy $E_{\text{c.m.}}=0.015\,808$ a.u., we observe, after a very short propagation time, an instantaneous loss of c.m. energy, which increases the

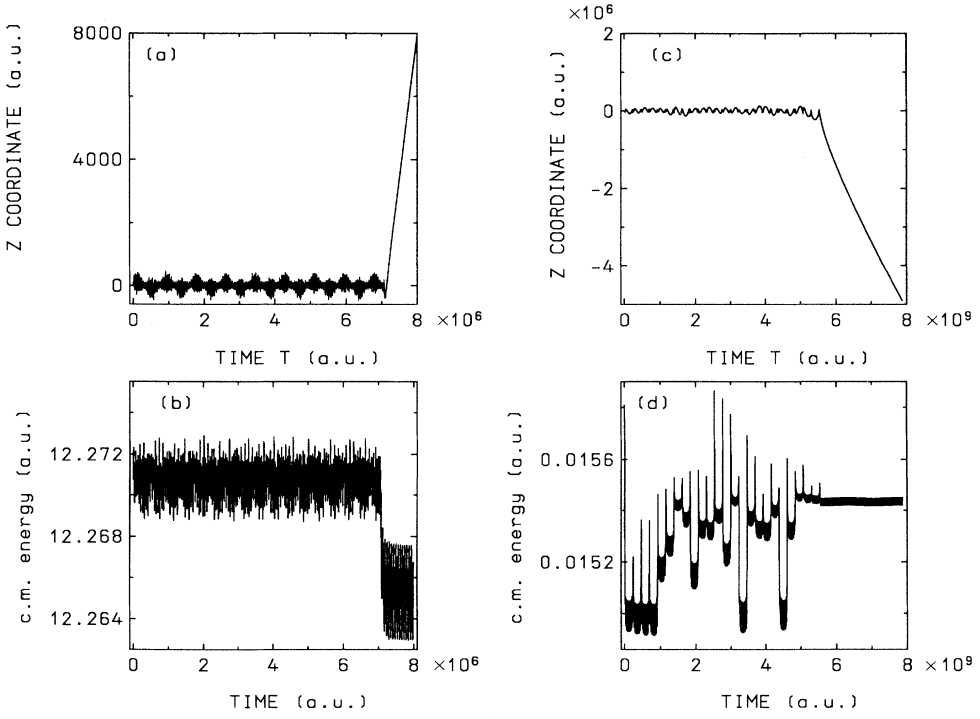

FIG. 4. (a) and (c) show the component of the relative coordinate parallel to the magnetic field as a function of time. (b) and (d) show the corresponding behavior of the c.m. energies. The parameter values are (a) and (b) $E_{\text{int}}=-3\times10^{-3}$, $B=10^{-4}$, and $E_{\text{c.m.}}=12.2707$ a.u. and (c) and (d) $E_{\text{int}}=-3.378\times10^{-4}$, $B=10^{-4}$, and $E_{\text{c.m.}}=1.581\times10^{-2}$ a.u. All values are given in atomic units.

internal energy above threshold. However, this time ionization does not occur immediately after the energy transfer has taken place. Instead we observe many further major steps of changes in the c.m. energy during which the internal energy is always above the escape threshold. To each such step there belongs a large amplitude oscillation in the electronic motion of the kind discussed in Sec. III C. Finally, after a propagation time of approximately 5.5×10^{9} a.u., ionization takes place. The ionization time therefore depends not only on the initial internal energy, the c.m. energy, and the field strength, but also on the intrinsic dynamics, which is, of course, covered by completely specifying the initial conditions of the individual trajectory. In the following we will investigate the statistics of the ionization process as a function of the c.m. and the internal energies.

In order to obtain a statistical measure for the ionization process, we have calculated, for an ensemble of trajectories, the fraction of ionized orbits as a function of time. The initial internal energy was chosen to correspond to a completely chaotic phase space of the He^{+} ion if the nuclear mass were infinite. The initial conditions for the internal motion have been selected randomly on the energy shell. In Fig. 5 we have illustrated the fraction of ionized orbits as a function of time up to $T=10^{10}$ a.u. for a series of different c.m. energies and for a fixed laboratory field strength of $B=10^{-4}$ a.u. For an initial c.m. energy of $E_{\text{c.m.}}=0.053$ a.u., which corresponds to an initial c.m. velocity of $V_{\text{c.m.}}=8.4\times10^{3}$ m s^{-1}, about 70% of the trajectories are ionized within a time of $T=10^{9}$ a.u. (2.4×10^{-8} s), which is the tenth part of the integration time. In contrast to this we have, for $E_{\text{c.m.}}=0.01$ a.u., only about 30% of ionized orbits within the total integration time of $T=10^{10}$ a.u. (2.4×10^{-7} s). The ionization process therefore depends very sensitively on the initial c.m. kinetic energy of the ion.

For initial internal energies and field strengths that belong to the regular regime, much higher initial c.m. velocities are necessary to order to obtain a substantial ionization rate. For example, for an initial c.m. kinetic energy $E_{\text{c.m.}}=1$ a.u. ($V_{\text{c.m.}}=3.6\times10^{4}$ m s^{-1}) and an initial internal energy $E_{\text{int}}=-0.003$ a.u., about 13% of the trajectories are ionized within $T=10^{9}$ a.u., whereas for the same internal energy and $E_{\text{c.m.}}=4$ a.u. ($V_{\text{c.m.}}=7.25\times10^{4}$ m s^{-1}), about 80% of the orbits are ionized within the same time interval. The c.m. kinetic energy necessary to observe ionization increases rapidly with decreasing internal energy and also with decreasing strength of the external magnetic field.

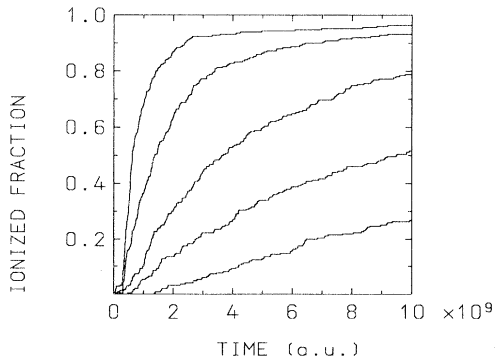

FIG. 5. Ionized fraction for an ensemble of 250 trajectories as a function of time. From top to bottom the c.m. energies belonging to the ionization curves are $E_{\text{c.m.}}=5.3\times10^{-2}$, 2.3×10^{-2}, 1.7×10^{-2}, 1.25×10^{-2}, and 10^{-2} a.u., respectively. The initial internal energy is always $E_{\text{int}}=-3.4\times10^{-4}$ a.u. The field strength is $B=10^{-4}$ a.u. All values are given in atomic units.

IV. SUMMARY AND CONCLUSIONS

In the presence of an external homogeneous magnetic field the c.m. and relative motion of an interacting particle system, such as a molecule or an atom, cannot be separated. The residual coupling of the collective and the internal motion is qualitatively different for neutral and charged systems. In the present paper we have investigated the effects and phenomena arising due to this coupling in the classical dynamics of a charged two-body system and in particular of the He^{+} ion. We thereby distinguished between the regular, the chaotic, and the intermittent regimes which are characterized by certain ranges of the parameter values (field strength, energy, etc.).

For regular phase space and vanishing initial c.m. velocity we observed four different (by orders of magnitude) time scales in the c.m. motion. On the largest time scale the effect of a *self-stabilization of the c.m. of the ion* on an approximately circular orbit is observed. The origin of this effect and of the different dynamical time scales is the coupling Hamiltonian of the c.m. and the electronic degrees of freedom, which causes an oscillating flow of energy between the collective and the internal motion. By using a pseudoparticle picture and averaging over the fast electronic degrees of freedom we were able to derive explicit expressions for the radius, the angular frequency, and the mean kinetic energy for the long-time circular c.m. motion. In the case of chaotic dynamics and vanishing initial c.m. velocity, the c.m. motion looks, on a short-time scale, very much like a random unbounded motion. On the long-time scale we obtained severe deviations of the collective motion from the circular motion observed in the regular regime: the circular shape was strongly disturbed even with one cycle and the c.m. left the circular orbit completely within a few cycles.

The classical dynamics becomes even more interesting if we increase the initial c.m. velocity. For total energies slightly above threshold and initial internal energies (field strengths, etc.) that correspond to a completely chaotic phase space we observe as a characteristic phenomenon the intermittent dynamics of the c.m. as well as the internal motion. Due to a sudden strong energy transfer from the c.m. to the electronic degrees of freedom and vice versa, alternating phases of quasiregular and chaotic motion are induced in the c.m. as well as the electronic motion.

The most prominent effect occurs if the c.m. energy is much larger than the absolute value of the internal energy of the ion. After a transient time of bound oscillations

in the internal motion (energy) a strong flow of energy from the c.m. to the internal motion takes place. The internal energy is hereby increased above the threshold for ionization and the ion eventually ionizes, i.e., the electron escapes in the direction parallel to the magnetic field. This *self-ionization effect* has been studied in some detail by considering the fraction of ionized orbits as a function of time for an ensemble of trajectories. The ionization process depends very sensitively on the initial c.m. kinetic energy and the initial internal energy.

All the considered values for the initial internal energy correspond to highly excited Rydberg states of the He^+ ion in a strong laboratory magnetic field. For sufficiently high excited electronic states the perturbation due to the coupling Hamiltonian of the c.m. and electronic degrees of freedom becomes larger than the spacing of adjacent levels due to the electronic Hamiltonian. As a consequence, strong mixing of the electronic and the c.m. wave functions occurs. In Ref. [12] estimations were given for the regime where this strong mixing occurs. In particular, this quantum regime of mixing includes the above-discussed classical regime for which we observe the process of self-ionization of the ion. In addition, since we are dealing with highly excited states for which the action is much larger than the elementary quantum of action, it seems probable that the self-ionization mechanism of the ion survives quantization. In the latter case this should have implications on different areas of physics such as plasma or astrophysics for which the stability of highly excited ions in strong magnetic fields in particular at finite temperatures is a relevant question.

The self-ionization effect should also be observable in laboratory experiments on fast moving ions in magnetic fields. In order to observe the effects of the coupling between the c.m. and the electronic motion, the following experiment is suggested. A fast beam of atomic ions has to be injected in a homogeneous magnetic field and subsequently the ions are excited by photons whose appropriately chosen frequency is below the threshold energy for ionization. Nevertheless, ionization, i.e., electron emission in the direction parallel to the magnetic field, should be observable by transfer of energy from the c.m. to the electronic motion. The typical electromagnetic decay time of the Rydberg states of the ion is of the same order of magnitude as our typical ionization times and they are therefore competing processes. By varying the field strength and/or c.m. velocity it is achievable that one or the other process dominates.

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APPENDIX

In the following we briefly discuss our transformations of the Newtonian equations of motion (5a), (5b), and (6). The main problem we are concerned with is to regularize the singularity that occurs due to the Coulomb potential in the equation of motion (5b). From celestial mechanics it is well known that the general two-body problem can be regularized and smoothened via the Kustaanheimo-Stiefel transformation [16]. We will take advantage of this well established transformation for our nonseparable charged two-body system in a magnetic field.

In a first step we introduce a fictitious time parameter s, which replaces the physical time t and is defined by

$$\frac{ds}{dt}=\frac{1}{r} , \tag{A1}$$

where r is the absolute value of the relative vector $\mathbf{r}$ of the two particles. After rewriting Eqs. (5a), (5b), and (6) as a system of differential equations with respect to the fictitious time we extend the relative vector $\mathbf{r}$ to a four-dimensional coordinate vector $\mathbf{x}$ by adding a vanishing fourth component. Subsequently we transform to a four-dimensional parameter space via the relation

$$\mathbf{x}=\mathcal{L}(\mathbf{u})\mathbf{u} , \tag{A2}$$

where $\mathcal{L}(\mathbf{u})$ is the Kustaanheimo-Stiefel matrix, a four-dimensional generalization of the Levi-Civita matrix

$$\mathcal{L}(\mathbf{u})=\begin{pmatrix} u_1 & -u_2 & -u_3 & u_4 \\ u_2 & u_1 & -u_4 & -u_3 \\ u_3 & u_4 & u_1 & u_2 \\ u_4 & -u_3 & u_2 & -u_1 \end{pmatrix} ,$$

and $\mathbf{u}^T=(u_1,u_2,u_3,u_4)$ is the vector in parameter space. Using the equations of motion for the internal energy with respect to the fictitious time s and in particular the translation of Eq. (6) to the fictitious time we arrive, after some algebra and repeated application of the transformation law (A2), at the final equations of motion

$$u''-\frac{1}{2\mu}h\mathbf{u}+\frac{e}{2\mu}\mathcal{L}^T(\mathbf{u})\mathbf{B}\times(\beta\mathbf{r}'+\alpha\mathbf{R}')=\mathbf{0} , \tag{A3}$$

$$h'=\frac{e\alpha}{M}\mathbf{B}\times(Q\mathbf{B}\times\mathbf{R}+e\alpha\mathbf{B}\times\mathbf{r}-\mathbf{K})\mathbf{r}' , \tag{A4}$$

where $\beta=(M_0^2-Zm^2)/M^2$ and the prime denotes the derivative with respect to the parameter s. $\mathbf{r}$ and $\mathbf{r}'$ in Eqs. (A3) and (A4) have to be substituted by the corresponding components of Eq. (A2) and the components of the identity

$$\mathbf{x}'=2\mathcal{L}(\mathbf{u})\mathbf{u}' , \tag{A5}$$

respectively. $\mathbf{x}'$ is the four-dimensional analog of $\mathbf{r}'$ with a vanishing fourth component. h is the internal energy and reads in parameter space as

$$h=(\mathbf{uu})^{-1}[2\mu(\mathbf{u}'\mathbf{u}')-Ze^2] . \tag{A6}$$

In addition, we have the equation of motion that arises from Eq. (6)

$$\mathbf{R}'=-\frac{(\mathbf{uu})}{M}(Q\mathbf{B}\times\mathbf{R}+e\alpha\mathbf{B}\times\mathbf{r}-\mathbf{K}) , \tag{A7}$$

where again $\mathbf{r}$ has to be replaced by the corresponding components of Eq. (A2). Our working equations (A3)–(A5) together with (A7) are smooth and free of any

singularities. The physical time can be obtained by simultaneous integration of Eq. (A1).

As a numerical integration algorithm for the above equations of motion we used a Bulirsch-Stoer integrator, which proved to be very fast for the smoothened equations of motion. In addition, due to the large step size of the integrator, it was possible to obtain an extremely high accuracy. For example, in the deep regular regime we obtained, after the integration of 10^4 Kepler cycles, still the impressive overall accuracy of 10^{-8}.

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