PHYSICAL REVIEW A VOLUME 54, NUMBER 6 DECEMBER 1996

Highly excited charged two-body systems in a magnetic field: A perturbation theoretical approach to classical dynamics

W. Becken and P. Schmelcher
Theoretische Chemie, Physikalisch-Chemisches Institut, Im Neuenheimer Feld 253, 69120 Heidelberg, Federal Republic of Germany
(Received 4 January 1996)

We investigate classical dynamics and properties of highly excited charged two-body systems in a magnetic field. We hereby focus on the regular regime which can be described by perturbation theoretical methods. After introducing the exact constants of motion as canonical momenta we apply a perturbation theoretical series expansion with respect to the parameter $\sigma := B^{1/2}$ and use a time-averaging method to obtain the long-time dynamical behavior of the system. This procedure allows us to identify approximate constants of motion and enables us to derive effective Hamiltonians which describe the averaged dynamics on different time scales. The doubly averaged equations of motion are in fourth-order perturbation theory integrable. The solutions of these equations in terms of rotators and librators are given analytically and phase space is classified completely. Finally we arrive at a thorough understanding of the recently found self-stabilization effect of the center-of-mass motion of the ion in the context of our perturbation theoretical investigation. [S1050-2947(96)07612-3]

PACS number(s): 32.60.+i, 47.20.Ky, 31.50.+w

I. INTRODUCTION AND PHENOMENA

The behavior of few-body systems in strong external fields became during the past twenty years a very active research field. The most thoroughly studied system is certainly the hydrogen atom in a strong magnetic field (see Ref. [1] and references therein). Both theoretically as well as experimentally large parts of the spectrum below as well as above the field-free ionization threshold [2] have been investigated in detail. The hydrogen atom in a magnetic field serves as an outstanding simple example of a physical system whose classical counterpart undergoes with increasing electronic excitation a transition from regularity to chaos. At the same time the properties of the atom change, with increasing action, from purely quantal to semiclassical and eventually to classical behavior.

In the presence of an external magnetic field, neutral as well as charged two-body systems possess an inherent two-body character, i.e., the center of mass (CM) and relative motion cannot be separated but are intimately coupled [3,4]. There exists, however, a constant of motion, the so-called pseudomomentum, which can be used to perform a pseudoseparation of the CM and relative motion. For neutral systems the components of this pseudomomentum are independent and the pseudoseparation accomplishes a complete elimination of the CM coordinates from the Hamiltonian [3–5]. Nevertheless, the CM and relative motion remain coupled and, in particular, the CM velocity is completely determined by the relative coordinates perpendicular to the magnetic field. Recently a number of two-body effects due to this coupling have been found and investigated for neutral systems [6–10]. As examples we mention the classical diffusion of the CM for chaotic phase space, the intermittent near-threshold dynamics of the CM as well as electronic motion and the existence of an outer potential well for sufficiently large pseudomomentum which yields a new class of weakly bound states with large electric dipole moments.

For the case of a system with a net charge Q the two components of the pseudomomentum perpendicular to the magnetic field do not commute and, therefore, they cannot be introduced simultaneously as canonical momenta. There exists, however, a generalization of the pseudoseparation for neutral systems to the case of a charged particle system [4,11–13]. The resulting Hamiltonian consists of three parts describing qualitatively different types of motion and couplings. The first part involves only CM degrees of freedom and treats the CM as a free pseudoparticle with charge Q and mass M (M is the total mass of the ion) in a magnetic field. The second part couples the CM and relative degrees of freedom and represents a motional Stark term with a rapidly oscillating electric field of intrinsic dynamical origin. This term arises due to the fact that a moving ion in a magnetic field experiences an additional electric field. Finally the third term involves only relative degrees of freedom, i.e., represents the electronic Hamiltonian for the case of an atom.

Very recently interesting effects and phenomena due to the coupling of the CM and electronic motions in one-electron atomic ions have been observed and studied [14]. The corresponding investigations have been performed by evaluating the results of the integration of the classical equations of motion for electronically highly excited atomic ions and are supported by quantum-mechanical considerations [12]. Two major effects have been reported: the self-stabilization and self-ionization effects. For regular CM and relative motion and vanishing initial CM velocity the self-stabilization of the highly excited ion on a cyclotron orbit takes place. For large values of the initial CM velocity the energy transfer from the CM to the electronic degrees of freedom becomes strong enough to allow the atom to ionize. The dynamical self-ionization process has been studied in some detail. Both the self-stabilization as well as the self-ionization effect are consequences of the presence of the coupling term between the CM and the electronic degrees of freedom. The self-stabilization effect has only been understood to some heuristic degree by performing an empirical averaging of the relevant quantities over the numerically observed different time scales of motion.

Since the self-stabilization effect takes place in the regular regime which is the subject of investigation of the present paper we provide in the following a few more details on the numerically observed classical behavior of the highly excited ion in this regime. We are referring to the case for which the Coulomb interaction dominates over the magnetic forces. In particular, let us concentrate on a vanishing initial CM velocity. In the absence of a magnetic field the ion would simply stay at rest. In the presence of a magnetic field, however, the above-mentioned coupling term causes an oscillating flow of energy between the CM and electronic degrees of freedom and the CM motion exhibits a variety of possibilities for its dynamical behavior. Four time scales, differing by orders of magnitude, have been observed for the CM motion. On the longest time scale the CM performs approximately a circular motion which corresponds to the motion of a free pseudoparticle with charge Q and mass M in a magnetic field. In spite of the fact that the initial CM velocity of the ion is equal to zero we encounter on this longest time scale the effect of self-stabilization of the ion on a cyclotron orbit. With the help of the above-mentioned empirical averaging procedure approximate expressions for the radius as well as the angular frequency of these orbits have been derived. We remark that the effect of the classical self-stabilization is a generic phenomenon for regular phase space and will in the following be shown to occur for any initial conditions.

The purpose of the present paper is the investigation of the regular regime for highly excited atomic ions in magnetic fields within the framework of classical perturbation theory. Apart from an improvement of our general understanding of the dynamics in the regular regime, our goals are to derive low-dimensional effective Hamiltonian equations of motion which describe the averaged classical motion on the different time scales, to reveal approximate constants of motion and, particularly, to gain a deeper understanding of the classical self-stabilization effect which has been observed in numerical simulations. In detail we proceed as follows. In Sec. II we perform, step by step, the canonical transformations of the Hamiltonian which introduce all existing exact constants of motion as canonical momenta, thereby eliminating the corresponding cyclic coordinates. Our choice of canonical variables and transformations already take into account the type of perturbation theory we want to apply. Appendixes A and B provide the necessary transformation formulas for the canonical CM and action angle variables of the Kepler problem. Section III gives a brief account of the perturbation theoretical ideas. Appendix C provides the general perturbation theoretical methods, i.e., the series expansion as well as the time-averaging procedure for the derivation of effective Hamiltonian and their equations of motion. In Sec. IV we apply the methods described in Appendix C to our case of the charged two-body system in a magnetic field. Many properties of the regular regime are derived and discussed.

II. CONSTANTS OF MOTION AND CANONICAL TRANSFORMATIONS OF THE HAMILTONIAN

Our starting point is the Hamiltonian for a charged two-body system of two interacting particles in a homogeneous external magnetic field

$$H'(\{\mathbf{p}'^{(i)}\},\{\mathbf{r}'^{(i)}\})=\sum_{i=1}^{2}\frac{1}{2m_i}[\mathbf{p}'^{(i)}-q_i\mathbf{A}(\mathbf{r}'^{(i)})]^2+V(|\mathbf{r}'^{(1)}-\mathbf{r}'^{(2)}|), \qquad (1)$$

where we have used the prime to label the quantities in the laboratory coordinate system. Throughout the paper we will use the symmetric gauge $\mathbf{A}(\mathbf{r})=\frac{1}{2}\mathbf{B}\times\mathbf{r}$ for the vector potential and the magnetic-field vector $\mathbf{B}$ along the z axis. In the following we perform a number of canonical transformations which will finally lead us to canonical variables which take into account all exact constants of motion and are best suited for a perturbation theoretical approach to the system. It is elucidating to perform these transformations step by step and not by a single composed canonical transformation: this way will provide us with a number of additional insights into the structure and properties of the underlying Hamiltonian as well as motivate our choice of variables for the perturbation theoretical approach.

In the absence of a magnetic field the total canonical (=kinetic) momentum is conserved and the straightlined uniform CM motion separates completely from the relative motion. The Kepler-Hamiltonian $H'^{[3]}$ involving the relative degrees of freedom is integrable and the commonly used action-angle variables are

$$I_1(\mathbf{p}',\mathbf{r}')=l'_z=x'p'_y-y'p'_x,$$

$$I_2(\mathbf{p}',\mathbf{r}')=|\mathbf{l}'|=\sqrt{(\mathbf{r}'\times\mathbf{p}')^2},$$

$$I_3(\mathbf{p}',\mathbf{r}')=\left(-\frac{\mu k^2}{2H'^{[3]}(\mathbf{p}',\mathbf{r}')}\right)^{1/2}, \qquad (2)$$

where $\mu=(m_1m_2/M)$ and k is the coupling constant of the (Coulomb) potential V. The dynamics is, in these variables, extremely simple, i.e., the action variables I_1,I_2,I_3 are conserved, the angles Φ_1, Φ_2 are constant, and Φ_3 shows a linear time dependence. As we shall see later on, part of these variables is also useful for the case of the presence of a magnetic field to which we shall turn next.

The Hamiltonian depends now on the vector potential A and therefore translations in space do not provide a symmetry. Instead the Hamiltonian is invariant with respect to the phase-space translation group [3]. The generators of this group are the components of the so-called pseudomomentum which is a conserved quantity and takes on the following appearance:

$$\mathbf{K}'=\sum_{i=1}^{2}\left(\mathbf{p}'^{(i)}+\frac{q_i}{2}\mathbf{B}\times\mathbf{r}'^{(i)}\right). \qquad (3)$$

The component K'_z is identical to the corresponding component of the total canonical momentum in field-free space and reflects the fact that the translation motion parallel to the magnetic field is uniform. If the net charge of the system is nonzero the components of the pseudomomentum perpendicular to the magnetic field do not commute and, therefore, cannot be used simultaneously in a complete set of constants of motion.

In addition the total canonical angular momentum parallel to the magnetic field

$$L_z' = \sum_{i=1}^{2} x'^{(i)} p_y'^{(i)} - y'^{(i)} p_x'^{(i)} \tag{4}$$

is conserved [15]. A maximal set of commuting constants of motion is $(H', \mathbf{K}_\perp'^2, K_z', L_z')$. In the following we will introduce, apart from field-dependent factors (see below), these quantities through canonical transformations as canonical momenta and will at the same time transform the remaining degrees of freedom to action-angle variables which are well suited for the perturbation theoretical approach with respect to the magnetic field.

In a first step we make the usual coordinate change from the laboratory coordinate system to CM variables $(\mathbf{R}_{\mathrm{cm}}, \mathbf{P}_{\mathrm{cm}})$ relative variables $(\mathbf{r}, \mathbf{p})$. In the latter coordinate frame the quantities K_z' and L_z' separate, i.e., are direct sums of different parts involving only CM and relative variables. The quantity $\mathbf{K}_\perp'^2$, however, does not separate in this sense. To achieve its separation the following unitary gauge transformation is necessary [4,11–13]:

$$\mathbf{P}_{\mathrm{cm}} = \mathbf{P}_{\mathrm{cm}}' + \frac{\beta}{2}\mathbf{B}\times\mathbf{r}',$$

$$p = p' - \frac{\beta}{2} B \times R_{\mathrm{cm}}', \tag{5}$$

where $\beta = [(q_1 m_2 - q_2 m_1)/M]$. The resulting Hamiltonian reads as follows:

$$H = H^{[1]} + H^{[2]} + H^{[3]},$$

$$H^{[1]} = \frac{1}{2M}\left(\mathbf{P}_{\mathrm{cm}} - \frac{Q}{2}\mathbf{B}\times\mathbf{R}_{\mathrm{cm}}\right)^2,$$

$$H^{[2]} = -\frac{\beta}{M}\left(\mathbf{P}_{\mathrm{cm}} - \frac{Q}{2}\mathbf{B}\times\mathbf{R}_{\mathrm{cm}}\right)\mathbf{B}\times\mathbf{r},$$

$$H^{[3]} = \frac{p^2}{2\mu} + \gamma_L B l_z + \lambda B^2(x^2+y^2) + V(r), \tag{6}$$

where l_z is the z component of the canonical relative angular momentum and

$$\gamma_L = \left(-\frac{q_1}{2m_1} - \frac{q_2}{2m_2} + \frac{Q}{2M}\right)$$

$$\lambda = \frac{1}{8}\left\{\frac{q_1^2}{m_1} + \frac{q_2^2}{m_2} - \frac{2Q}{M^2}(q_1 m_1 + q_2 m_2) + Q^2\frac{m_1^3 + m_2^3}{M^4}\right\}. \tag{7}$$

It has a particular appealing form which has been mentioned in the introduction. $H^{[1]}$ is the CM Hamiltonian for a free pseudoparticle with charge Q and mass M in a magnetic field which treats the ion as an entity. $H^{[2]}$ contains the coupling of the CM and relative degrees of freedom and represents a motional Stark term with a rapidly oscillating electric field of intrinsic dynamical origin. $H^{[3]}$ is the purely electronic Hamiltonian. With the above transformation we have achieved even more than we wanted: $\mathbf{K}_\perp^2$ depends now solely on the CM variables, i.e., $\mathbf{K}_\perp^2 = \mathbf{K}_{\mathrm{cm}\perp}^2$! (The reader should carefully distinguish between the total quantities $\mathbf{K}_\perp^2$, $\mathrm{L_z}$ and the CM variables $\mathbf{K}_{\mathrm{cm}\perp}^2, L_{\mathrm{cm}z}$ which are, in general, different quantities.) This means that we are now ready to introduce, by a further canonical transformation, $\mathbf{K}_\perp^2$ as a canonical momentum (see also Ref. [17]). The complete set of new canonical momenta for the CM variables, i.e., for the Hamiltonian $H^{[1]}$, are

$$(p_1, p_2, p_3) = \left(\frac{\mathbf{K}_{\mathrm{cm}\perp}^2}{2B}, L_{\mathrm{cm}z}, P_{\mathrm{cm}z}\right).$$

With these momenta the Hamiltonian $H^{[1]}$ reads

$$H^{[1]} = \frac{p_3^2}{2M} + B\left(\gamma_Z p_2 + \frac{p_1}{M}\right), \tag{8}$$

with $\gamma_Z := -(Q/M)$. For the corresponding canonical conjugated coordinates (q_1, q_2, q_3) we refer the reader to Appendix A. Since $H^{[1]}$ is integrable it depends only on the conserved momenta p_i. We included a factor $1/2B$ in the definition of the canonical momentum p_1 due to the following reason: after the canonical transformation to the momenta p_i the relevant part of the Hamiltonian $H^{[1]}$ [see Eq. (8)] consists only of terms which are linear proportional to the magnetic-field strength [this is not the case for the corresponding Hamiltonian in Eqs. (6) which contains terms proportional to B as well as B^2]. Equally important, the coupling Hamiltonian $H^{[2]}$ will, in the above-chosen scaled variables, also be proportional to only one power of the field strength, namely, to $B^{3/2}$ [see Eq. (10)]. These facts are of particular relevance and desirable for our later on perturbation theoretical expansion in terms of powers of the magnetic-field strength since we will be able to take into account the CM or coupling Hamiltonian by the inclusion of a single low perturbation theoretical order in the field strength. We remark that this scale transformation does not prevent us from performing a consistent perturbation theory. Since the only rescaled variable p_1 is a constant of motion, every rescaled expression in the equations of motion appears only in connection with this conserved quantity and therefore does not affect the dynamics of our perturbation theory. For any field strength and, in particular, for the low-field limit $B \to 0$, the above-performed scaling does not cause any intricacies. Before the limit $B \to 0$ is performed the constant $p_1 = (\mathbf{K}_{\mathrm{cm}\perp}{}^2/2B)$ has to be reinserted and will only occur in connection with an additional multiplicative power of the field strength which makes the limiting process smooth.

We mention that a transformation to a coordinate system rotating around the magnetic-field axis would yield an explicitly time-dependent coupling Hamiltonian $H^{[2]}$ which is difficult to handle in our perturbation theoretical approach.

For the internal Hamiltonian $H^{[3]}$ we choose the action angle variables of the Kepler problem [see Eqs. (2)] as the new variables [see also Ref. [16]] and arrive after some lengthy algebra (see Appendix B for the corresponding transformation formulas) at

$$H^{[3]}(I,\Phi)=-\frac{\mu k^2}{2I_3^2}+\gamma_L BI_1+\lambda B^2\,\frac{I_2^4}{\mu^2k^2}\times\frac{\left[1-\sin^2[\chi(I_2,I_3,\phi_3)+\phi_2]\left(1-\frac{I_1^2}{I_2^2}\right)\right]}{[1+\epsilon(I_2,I_3)\cos\chi(I_2,I_3,\phi_3)]^2}. \tag{9}$$

The functions $\epsilon(I_2,I_3)$, $\chi(I_2,I_3,\phi_3)$ are given in Appendix B. $H^{[3]}$ does not depend on ϕ_1 which reflects the fact that it conserves the canonical relative angular momentum component parallel to the magnetic field. Finally the coupling Hamiltonian $H^{[2]}$ takes on the following appearance:

$$H^{[2]}=-\frac{\sqrt{2}\beta}{M}\,B^{3/2}\sqrt{p_1-Qp_2}\;r(I_2,I_3,\phi_3)\times\Big(\sin(q_2-\phi_1)\cos(\phi_2+\chi)-\cos(q_2-\phi_1)\times\sin(\phi_2+\chi)\,\frac{I_1}{I_2}\Big), \tag{10}$$

where $r(I_2,I_3,\phi_3)$ is also given in Appendix B. The coupling Hamiltonian $H^{[2]}$ depends on ϕ_1 and, therefore, does not conserve the angular momentum I_1. This had to be expected since the total Hamiltonian H does not conserve the relative angular momentum I_1 but the total angular momentum L_z! The conservation of L_z can be seen from Eq. (10) by its dependence on $(q_2-\phi_1)$ and not on q_2 or ϕ_1 separately. Our last canonical transformation which introduces in addition to the other conserved quantities also L_z, or more precisely $L_z/2$, as a canonical conjugated momentum reads as follows:

$$\mathcal{L}=\tfrac{1}{2}(p_2+I_1),\quad \xi=q_2+\phi_1$$
$$\overline{\mathcal{L}}=\tfrac{1}{2}(p_2-I_1),\quad \overline{\xi}=q_2-\phi_1. \tag{11}$$

Using this canonical transformation we arrive at the following appearance of our final Hamiltonian:

$$H(\mathcal{L},p_1,p_3;\overline{\mathcal{L}},I_2,I_3,\overline{\xi},\phi_2,\phi_3)=H^{[1]}(\mathcal{L},p_1,p_3;\overline{\mathcal{L}})+H^{[2]}(\mathcal{L},p_1;\overline{\mathcal{L}},I_2,I_3,\overline{\xi},\phi_2,\phi_3)+H^{[3]}(\mathcal{L};\overline{\mathcal{L}},I_2,I_3,\phi_2,\phi_3), \tag{12}$$

with

$$H^{[1]}(\mathcal{L},p_1,p_3;\overline{\mathcal{L}})=\frac{p_3^2}{2M}+B\left(\gamma_Z(\mathcal{L}+\overline{\mathcal{L}})+\frac{p_1}{M}\right), \tag{13}$$

$$H^{[2]}(p_1,\mathcal{L};\overline{\mathcal{L}},I_2,I_3,\overline{\xi},\phi_2,\phi_3)=-\frac{\sqrt{2}\beta}{M}\,B^{3/2}\sqrt{p_1-Q(\mathcal{L}+\overline{\mathcal{L}})}\;r(I_2,I_3,\phi_3)\times\left(\sin\overline{\xi}\cos(\phi_2+\chi)-\cos\overline{\xi}\sin(\phi_2+\chi)\,\frac{\mathcal{L}-\overline{\mathcal{L}}}{I_2}\right), \tag{14}$$

$$H^{[3]}(\mathcal{L};\overline{\mathcal{L}},I_2,I_3,\phi_2,\phi_3)=-\frac{\mu k^2}{2T_3^2}+\gamma_L B(\mathcal{L}-\overline{\mathcal{L}})+\lambda B^2 r^2(I_2,I_3,\phi_3)\times\left[1-\sin^2(\chi+\phi_2)\left(1-\frac{(\mathcal{L}-\overline{\mathcal{L}})^2}{I_2^2}\right)\right]. \tag{15}$$

The arguments of the Hamiltonian are the conserved momenta separated by a semicolon from the dynamical variables. Our final total Hamiltonian H in Eq. (12) is only a function of the momenta $(p_1,p_3,\mathcal{L},\mathcal{L},I_2,I_3)$ and of the coordinates (ξ,ϕ_2,ϕ_3). The coordinates q_1,q_3,ξ are cyclic since their corresponding momenta $p_1,p_3,\mathcal{L}$ are conserved. The motion of the cyclic coordinates q_1,q_3,ξ separates from the motion of the coupled dynamical variables $(\mathcal{L},I_2,I_3,\xi,\phi_2,\phi_3)$ in the sense that the motion of the set of cyclic coordinates can be calculated independently and one by one after solving the coupled Hamiltonian equations of motion for the set $(\mathcal{L},I_2,I_3,\xi,\phi_2,\phi_3)$ of variables. We remark that once the dynamical behavior of ξ is known the time dependence of the second nontrivial cyclic coordinate q_1 can be easily obtained by using the equation of conservation for the pseudomomentum.

Let us conclude. By performing several canonical transformations we arrived at a particularly simple and appealing form for the Hamiltonian of a one-electron ion in a magnetic field. The conserved quantities

$$\left(\frac{\mathbf{K}_\perp^2}{2B},K_z,\ \frac{L_z}{2}\right)$$

have been introduced as canonical momenta and we hereby reduced the number of coupled dynamical degrees of freedom from six to three, i.e., we reduced the coupled phase space from 12 to 6 dimensions. Secondly, by choosing the above field-dependent scale transformation the pure CM part as well as the coupling part of the total Hamiltonian became proportional to a single low power of the field strength. We have, therefore, obtained a very good starting point for a perturbation theoretical treatment of the classical (and in the future also semiclassical) dynamics of highly excited ions in external magnetic fields and turn next to a brief description of our perturbation theoretical approach.

III. PERTURBATION THEORETICAL CONCEPTS

Our unperturbed Hamiltonian is the Kepler-Hamiltonian in field-free space and the perturbation expansion will be done in powers of the magnetic-field strength. In spite of the fact that our example of application will be the He^+ ion all following considerations and perturbation theoretical results are valid for any mass ratio of the two particles. We mention that the special case of an infinite nuclear mass which corresponds to the Hamiltonian $H^{[3]}$ for $m_2\to\infty$ has been investigated in detail in Ref. [16]. The perturbation theoretical approach to the hydrogen atom in crossed electric and magnetic fields has been developed in Ref. [18–20]. If we rearrange the total Hamiltonian H in terms of powers of the magnetic-field strength we immediately realize that the perturbation theoretical expansion parameter is best chosen as $\sigma:=B^{1/2}$, since the coupling Hamiltonian $H^{[2]}$ is proportional to $B^{3/2}$. Our expanded Hamiltonian, therefore, looks as follows:

$$H(\mathcal{L},p_1,p_3;\overline{\mathcal{L}},I_2,I_3,\overline{\xi},\phi_2,\phi_3) = H_0(p_3;I_3)+\frac{\sigma^2}{2!}H_2(\mathcal{L},p_1;\overline{\mathcal{L}}) + \frac{\sigma^3}{3!}H_3(\mathcal{L},p_1;\overline{\mathcal{L}},I_2,I_3,\overline{\xi},\phi_2,\phi_3) + \frac{\sigma^4}{4!}H_4(\mathcal{L};\overline{\mathcal{L}},I_2,I_3,\phi_2,\phi_3), \tag{16}$$

with

$$H_0(p_3;I_3)=\frac{p_3^2}{2M}-\frac{\mu k^2}{2I_3^2}, \tag{17}$$

$$H_2(\mathcal{L},p_1;\overline{\mathcal{L}})=2\left(\gamma\mathcal{L}+\frac{p_1}{M}\right)+2\overline{\gamma}\overline{\mathcal{L}} \tag{18}$$

$$H_3(\mathcal{L},p_1;\overline{\mathcal{L}},I_2,I_3,\overline{\xi},\phi_2,\phi_3) = -6\frac{\sqrt{2}\beta}{M}\sqrt{p_1-Q(\mathcal{L}+\overline{\mathcal{L}})}\frac{I_2^2}{\mu k}\frac{1}{1+\epsilon\cos\chi} \times\left(\sin\overline{\xi}\cos(\phi_2+\chi)-\cos\overline{\xi}\sin(\phi_2+\chi)\frac{\mathcal{L}-\overline{\mathcal{L}}}{I_2}\right), \tag{19}$$

$$H_4(\mathcal{L};\overline{\mathcal{L}},I_2,I_3,\phi_2,\phi_3)=24\lambda\frac{I_2^4}{\mu^2k^2}\frac{1}{(1+\epsilon\cos\chi)^2} \times\left[1-\sin^2(\chi+\phi_2)\times\left(1-\frac{(\mathcal{L}-\overline{\mathcal{L}})^2}{I_2^2}\right)\right], \tag{20}$$

with $\gamma:=\gamma_Z+\gamma_L$ and $\overline{\gamma}:=\gamma_Z-\gamma_L$. The zeroth-order Hamiltonian H_0 consists, apart from the trivial CM energy parallel to the magnetic field, of the pure Kepler-Hamiltonian. The Hamiltonian H_2 contains the complete cyclotron motion of the ion treated as a pseudoparticle with charge Q and mass M in a magnetic field as well as the Zeeman term of $H^{[3]}$. Since $p_1,\mathcal{L}$ are conserved momenta the only term in H_2 which contributes to the coupled part of the corresponding Hamiltonian equations of motion (see below) is the term involving the momentum $\overline{\mathcal{L}}$. Finally H_3 represents the coupling Hamiltonian between the CM and electronic motion and H_4 is the diamagnetic electronic part of $H^{[3]}$.

In Appendix C we give a brief account of our perturbation theoretical approach which will be applied in Sec. IV to the Hamiltonian (16). In order to establish the equations of motion for each order in σ, a series expansion due to the explicit and implicit dependence, for all relevant quantities (Hamiltonian and variables), on σ has to be performed. Because of the particular structure of the zeroth order and the exact Hamiltonian (see the beginning of Appendix C) our perturbation theoretical equations of motion can be simplified in each order enormously [see Eqs. (C9)–(C11)].

Apart from the perturbation theoretical approach with respect to σ there is another conceptual idea which will be used extensively in our investigation of the classical motion of the highly excited ion. According to the numerical simulations performed in Refs. [14] the CM as well as electronic motion exhibit several oscillatory motions on by-orders-of-magnitude different time scales T_i (whether, and if yes, how these time scales can be derived from the different parts of the expanded Hamiltonian H will be clarified in Sec. IV). These oscillatory motions are superimposed on each other. It is therefore a natural idea to obtain the motion on a larger time scale by averaging over the fast individual oscillations on the smaller time scale. This can successively be done until one arrives at a complete picture of the motion on any of the existing time scales. The shortest time scale, i.e., fastest oscillatory motion, is the one due to the time dependence of the angle ϕ_3 which represents in order σ^0 the period $\tau_K=(2\pi I_3^3/\mu k^2)$ of the Kepler ellipses. The second time scale is given by the oscillatory motion of the angle $\overline{\xi}$ which arises first for the order σ^2 and possesses in this order the period $\overline{\tau}=(2\pi/|\overline{\gamma}\sigma^2|)$. Up to order σ^2 our expanded Hamiltonian is integrable. It possesses no coupling between the CM and electronic degrees of freedom and describes the CM motion as a free cyclotron motion of a pseudoparticle with charge Q and mass M in a magnetic field and the electronic motion as Kepler ellipses which are rotating with their Larmor frequency.

The next higher order σ^3 of the perturbation expansion involves the coupling Hamiltonian H_3 which depends on the angles $\phi_3,\overline{\xi}$ (belonging to the above-mentioned time scales) and which destroys, in particular, the property of I_3 and $\overline{\mathcal{L}}$ being conserved quantities (see, however, Sec. IV). Since the exact solutions $\overline{\mathcal{L}}(t),I_2(t),I_3(t),\overline{\xi}(t),\phi_2(t),\phi_3(t)$ of the Hamiltonian equations of motion are unknown, the question for the practical feasibility of the time-averaging procedure now arises. Let us consider first the fastest oscillations due to the motion of ϕ_3. For a certain cycle of ϕ_3 the above unknown functions could in a first approximation be replaced in the Hamiltonian equations of motion by their initial values and the angle ϕ_3 by its linear time behavior due to the pure Kepler problem. The changes $\Delta\overline{\mathcal{L}},\Delta I_2,\Delta I_3,\Delta\overline{\xi},\Delta\phi_2,\Delta\phi_3$ after one time cycle τ_K then arise from the time averages of the quantities $\dot{\overline{\mathcal{L}}},\dot{I}_2,\dot{I}_3,\dot{\overline{\xi}},\dot{\phi}_2,\dot{\phi}_3$ and tell us the change in the above variables due to the coupling during one cycle as well as the deviation of the angle ϕ_3 from its uniform time dependence. Such a procedure yields a system of difference equations which can, under appropriate conditions, be replaced by a system of differential equations. These conditions demand, roughly speaking, the smallness of the second derivatives of all quantities. Corrections going beyond the described approximation for the averaging over the smallest time scale can be shown (see Appendix C and, in particular, Ref. [22]) to be of order σ^5 and are therefore within our perturbation theoretical approach of order σ^4 negligible. The smallest time scale of the averaged equations of motion is now $\overline{\tau}=(2\pi/|\overline{\gamma}|\sigma^2)$ due to the motion of ξ. To obtain the motion on even larger time scales one uses the fact that the variables $\mathcal{L},I_2,I_3,\phi_2$ are constant on the time scale $\overline{\tau}$ and performs a second averaging procedure now over the time scale $\overline{\tau}$. Corrections due to this second averaging are of order σ^4 and will be given in Sec. IV (see also Appendix C). The corrections of the second averaging process go together with the diamagnetic electronic term which occurs in the next order σ^4 of perturbation theory. They determine the behavior of the system on a time scale much larger than $\overline{\tau}$ and define, as we shall see, a third even longer time scale. For the mathematical details of the performance of the averaging procedure and for the corresponding notation we refer the reader to Appendix C and Ref. [22].

IV. RESULTS AND DISCUSSION

In the present section we apply the perturbation theoretical method to our problem of the charged two-body system in an external magnetic field. First of all we establish the exact perturbation theoretical equations of motion up to fourth order in σ, i.e., $r=4$. Let us begin by providing the first few perturbational theoretical Hamiltonian $H^{(r)}$ for the lowest orders $r\leqslant 4$ [see Eqs. (C3) and (C4) in Appendix C]. In zeroth order we obtain $H^{(0)}(p_3;I_{30})=H_0(p_3;I_{30})$ and the first-order contribution vanishes, i.e., $H^{(1)}=0$. In second order we have $H^{(2)}(\mathcal{L},p_1;\mathcal{L}_0)=H_2(\mathcal{L},p_1;\mathcal{L}_0)$, where $\mathcal{L}_0\equiv\mathcal{L}(0)$. Apart from that for $\xi(t)$, all solutions of second order vanish. For the third and fourth order we obtain

$$
\begin{aligned}
&H^{(3)}(\mathcal{L},p_1;\overline{\mathcal{L}_0},I_{20},I_{30},\overline{\xi_0},\phi_{20},\phi_{30}|I_{33})\\
&\quad=H_3(\mathcal{L},p_1;\overline{\mathcal{L}_0},I_{20},I_{30},\overline{\xi_0},\phi_{20},\phi_{30})\\
&\qquad+I_{33}\frac{\partial}{\partial I_{30}}H_0(p_3;I_{30}),\\
&H^{(4)}(\mathcal{L};\overline{\mathcal{L}_0},I_{20},I_{30},\phi_{20},\phi_{30}|I_{33})\\
&\quad=H_4(\mathcal{L};\overline{\mathcal{L}_0},I_{20},I_{30},\phi_{20},\phi_{30})+I_{34}\frac{\partial}{\partial I_{30}}H_0(p_3;I_{30}).
\end{aligned}
\tag{21}
$$

The coupled part of the corresponding Hamiltonian equations of motion read in zeroth, second, third, and fourth order as follows:

$r=0$:

$$\dot{\phi}_{30}=\frac{\partial}{\partial I_{30}}H_0(I_{30}),\tag{22}$$

$r=2$:

$$\dot{\overline{\xi}}_2=\frac{\partial}{\partial\overline{\mathcal{L}_0}}H_2(\overline{\mathcal{L}_0}),\tag{23}$$

$r=3$:

$$
\begin{aligned}
\dot{\overline{\mathcal{L}}}_3&=-\frac{\partial}{\partial\overline{\xi_0}}H_3(\overline{\mathcal{L}_0},I_{20},I_{30},\overline{\xi_0},\phi_{20},\phi_{30}),\\
\dot{I}_{23}&=-\frac{\partial}{\partial\phi_{20}}H_3(\overline{\mathcal{L}_0},I_{20},I_{30},\overline{\xi_0},\phi_{20},\phi_{30}),\\
\dot{I}_{33}&=-\frac{\partial}{\partial\phi_{30}}H_3(\overline{\mathcal{L}_0},I_{20},I_{30},\overline{\xi_0},\phi_{20},\phi_{30}),\\
\dot{\overline{\xi}}_3&=\frac{\partial}{\partial\overline{\mathcal{L}_0}}H_3(\overline{\mathcal{L}_0},I_{20},I_{30},\overline{\xi_0},\phi_{20},\phi_{30}),\\
\dot{\phi}_{23}&=\frac{\partial}{\partial I_{20}}H_3(\overline{\mathcal{L}_0},I_{20},I_{30},\overline{\xi_0},\phi_{20},\phi_{30}),\\
\dot{\phi}_{33}&=\frac{\partial}{\partial I_{30}}H_3(\overline{\mathcal{L}_0},I_{20},I_{30},\overline{\xi_0},\phi_{20},\phi_{30})+I_{33}\frac{\partial^2}{\partial I_{30}^2}H_0(I_{30}),
\end{aligned}
\tag{24}
$$

$r=4$:

$$
\begin{aligned}
\dot{\overline{\mathcal{L}}}_4&=0,\\
\dot{I}_{24}&=-\frac{\partial}{\partial\phi_{20}}H_4(\overline{\mathcal{L}_0},I_{20},I_{30},\phi_{20},\phi_{30}),\\
\dot{I}_{34}&=-\frac{\partial}{\partial\phi_{30}}H_4(\overline{\mathcal{L}_0},I_{20},I_{30},\phi_{20},\phi_{30}),\\
\dot{\overline{\xi}}_4&=\frac{\partial}{\partial\overline{\mathcal{L}_0}}H_4(\overline{\mathcal{L}_0},I_{20},I_{30},\phi_{20},\phi_{30}),\\
\dot{\phi}_{24}&=\frac{\partial}{\partial I_{20}}H_4(\overline{\mathcal{L}_0},I_{20},I_{30},\phi_{20},\phi_{30}),\\
\dot{\phi}_{34}&=\frac{\partial}{\partial I_{30}}H_4(\overline{\mathcal{L}_0},I_{20},I_{30},\phi_{20},\phi_{30})+I_{34}\frac{\partial^2}{\partial I_{30}^2}H_0(I_{30}),
\end{aligned}
\tag{25}
$$

which shows that up to second order all canonical momenta are conserved. In addition the decoupled equations of motion for the variable ξ for the orders $r=2,3,4$ take on the following appearance:

$$
\begin{aligned}
\dot{\xi}_2&=\frac{\partial}{\partial\mathcal{L}}H_2(\mathcal{L},p_1;\overline{\mathcal{L}_0}),\\
\dot{\xi}_3&=\frac{\partial}{\partial\mathcal{L}}H_3(\mathcal{L},p_1;\overline{\mathcal{L}_0},I_{20},I_{30},\overline{\xi_0},\phi_{20},\phi_{30}),\\
\dot{\xi}_4&=\frac{\partial}{\partial\mathcal{L}}H_4(\mathcal{L};\overline{\mathcal{L}_0},I_{20},I_{30},\phi_{20},\phi_{30}).
\end{aligned}
\tag{26}
$$

The above perturbation theoretical equations now clearly reveal that the time scale τ_K of order $r=0$ belongs to the motion of ϕ_{30}, the time scales $\overline{\tau}=(2\pi/|\overline{\gamma}|\sigma^2)$ and $\tau=(2\pi/|\gamma|\sigma^2)$ of order $r=2$ belong to the motion $\overline{\xi}_2$ and ξ_2, respectively.

In order to study the behavior of the system on a long-time period we have to average the fast oscillations due to the variables ϕ_3 and $\overline{\xi}$. The underlying ideas and the formal aspects of this averaging procedure have been described in some detail in the preceding section and particularly in Appendix C. We, therefore, refer in the following only to the results of the corresponding calculations.

Let us begin with the averaging over the shortest time scale due to the rapid oscillatory motion of ϕ_3. The nth averaging period is the momentary Kepler period after $(n-1)$ cycles of ϕ_{30}, i.e., $\Delta T(n)=[2\pi I_3^3(n)/\mu k^2]$. In averaging Eqs. (22)–(26) we use the fact that all Hamiltonian are periodic with respect to ϕ_3 and can be represented in Fourier series according to Eq. (C13) in Appendix C. The corresponding Fourier components are provided in Appendix D. Subsequently we take the continuum limit of the resulting averaged difference equations and arrive at the following differential equations for the canonical averaged variables:

$$\frac{d\overline{\mathcal{L}}}{dT}=-\frac{\sigma^3}{3!}\frac{\partial H_{30}}{\partial\overline{\xi}},$$

$$\frac{dI_2}{dT}=-\frac{\sigma^3}{3!}\frac{\partial H_{30}}{\partial\phi_2}-\frac{\sigma^4}{4!}\frac{\partial H_{40}}{\partial\phi_2},$$

$$\frac{dI_3}{dT}=0,$$

$$\frac{d\overline{\xi}}{dT}=\frac{\sigma^2}{2!}\frac{\partial H_{20}}{\partial\overline{\mathcal{L}}}+\frac{\sigma^3}{3!}\frac{\partial H_{30}}{\partial\overline{\mathcal{L}}}+\frac{\sigma^4}{4!}\frac{\partial H_{40}}{\partial\overline{\mathcal{L}}},$$

$$\frac{d\phi_2}{dT}=\frac{\sigma^3}{3!}\frac{\partial H_{30}}{\partial I_2}+\frac{\sigma^4}{4!}\frac{\partial H_{40}}{\partial I_2} \tag{27}$$

and for the decoupled variables

$$\frac{d\phi_3}{dT}=+\frac{\sigma^3}{3!}\left(\frac{\partial H_{30}}{\partial I_3}+(*)\right)+\frac{\sigma^4}{4!}\left(\frac{\partial H_{40}}{\partial I_3}+(*)\right),$$

$$\frac{d\xi}{dT}=\frac{\sigma^2}{2!}\frac{\partial H_{20}}{\partial\mathcal{L}}+\frac{\sigma^3}{3!}\frac{\partial H_{30}}{\partial\mathcal{L}}+\frac{\sigma^4}{4!}\frac{\partial H_{40}}{\partial\mathcal{L}}, \tag{28}$$

where the asterisk symbolizes contributions which are not explicit derivative terms. We immediately realize the following important results of our averaging procedure. The averaged time derivatives of I_{33},I_{34} vanish and the first nonvanishing contribution to I_3 arises in fifth-order perturbation theory. The averaged variable I_3 is therefore in fourth order an exact constant of motion [see Eqs. (27)] and, in general, for the regime accessible by perturbation theory an *approximate constant of motion*.

Second, we observe that the terms representing derivatives do no more contain the Hamiltonian H_l, but their zeroth Fourier components H_{l0} with respect to ϕ_3, and these components, do not depend on ϕ_3. In particular, up to order $r=4$, ϕ_3 does not show up in the equations of motion for the coupled variables $(\mathcal{L},\xi)$, (I_2,ϕ_2) and the variables (I_3,ϕ_3), therefore, decouple in the averaged equations of motion. Consequently the number of coupled degrees of freedom is reduced by the averaging procedure from three to two. Another important property of the averaged coupled equations is the fact that they possess Hamiltonian structure which was not the case for the original perturbation theoretical equations of motion [see also Appendix C, in particular, Eqs. (C14) and below].

$$H_{\text{eff}}(\sigma;\mathcal{L},p_1,I_3;\overline{\mathcal{L}},I_2\overline{\xi},\phi_2)$$
$$:=\frac{\sigma^2}{2!}H_{20}(\mathcal{L},p_1;\overline{\mathcal{L}})+\frac{\sigma^3}{3!}H_{30}(\mathcal{L},p_1,I_3;\overline{\mathcal{L}},I_2,\overline{\xi},\phi_2)$$
$$+\frac{\sigma^4}{4!}H_{40}(\mathcal{L},I_3;\overline{\mathcal{L}},I_2,\phi_2), \tag{29}$$

with the Fourier components H_{20},H_{30},H_{40} given in Appendix D 1.

From Eqs. (22)–(25) we know that, apart from the fast oscillations of ϕ_3, there is a second larger time scale defined by the behavior of ξ. The effective Hamiltonian (29) is periodic with respect to the angle variable ξ. It is, therefore, an obvious idea to repeat the above-performed averaging procedure but now with respect to the variable ξ and its time scale. Before doing this according to the procedure described in Appendix C we have to meet the requirements given at the very beginning in Appendix C. This means, in particular, that the zeroth order of our Hamiltonian to be averaged over ξ should contain the fast oscillations of ξ. This can be accomplished by the rescaling of time $\vartheta:=\sigma^2\cdot T$ which yields a rescaling of the Hamiltonian H_{eff} by a factor of $1/\sigma^2$, i.e., $\mathcal{H}_{\text{eff}}=(1/\sigma^2)H_{\text{eff}}$ in the corresponding equations of motion. We remark that these scale transformations do not prevent us from performing a, up to some desired order, consistent perturbation theory. The coupled equations of motion read then as follows:

$$\frac{d\overline{\mathcal{L}}}{d\vartheta}=-\frac{\partial\mathcal{H}_{\text{eff}}}{\partial\overline{\xi}},$$

$$\frac{dI_2}{d\vartheta}=-\frac{\partial\mathcal{H}_{\text{eff}}}{\partial\phi_2},$$

$$\frac{d\overline{\xi}}{d\vartheta}=\frac{\partial\mathcal{H}_{\text{eff}}}{\partial\overline{\mathcal{L}}},$$

$$\frac{d\phi_2}{d\vartheta}=\frac{\partial\mathcal{H}_{\text{eff}}}{\partial I_2}. \tag{30}$$

Next we apply the procedure described in Appendix C to these equations, i.e., we expand them with respect to their total dependence on σ and average the resulting equations over the period $\Delta\Theta=2\pi/|\overline{\gamma}|$, where $\Theta=\sigma^2\mathcal{T}$ stands for the continuous scaled time variable after the second averaging process.

The resulting effective Hamiltonian can, after some lengthy calculation, be shown to possess the following structure:

$$\mathcal{H}_{\mathrm{eff}_{\mathrm{eff}}}(\sigma;\mathcal{L},p_1,I_3;\overline{\mathcal{L}};I_2,\phi_2)$$
$$:=\frac{\sigma^2}{2!}\Bigg(\mathcal{H}_{\mathrm{eff}_{20}}(\mathcal{L},p_1,I_3;\overline{\mathcal{L}},I_2,\phi_2)+\frac{2}{\mathcal{H}'_{\mathrm{eff}_{00}}}\sum_{k\neq 0}\left\{1/ik\,\frac{\partial\mathcal{H}_{\mathrm{eff}_{1k}}}{\partial I_2(\Theta)}\frac{\partial\mathcal{H}_{\mathrm{eff}_{1(-k)}}}{\partial\phi_2(\Theta)}-\mathcal{H}_{\mathrm{eff}_{1(-k)}}\frac{\partial\mathcal{H}_{\mathrm{eff}_{1k}}}{\partial\overline{\mathcal{L}}(\Theta)}\right\}\Bigg), \tag{31}$$

with the Fourier components $H_{\mathrm{eff}_{ij}}$ given in Appendix D 2. The first term arises due to the diamagnetic term and reads

$$\mathcal{H}_{\mathrm{eff}_{20}}(\mathcal{L},I_2,\phi_2)=\frac{\lambda}{2}\frac{1}{\mu^2k^2}\frac{I_3^2}{I_2^2}\big((5I_3^2-3I_2^2)[I_2^2+(\mathcal{L}-\overline{\mathcal{L}})^2]+5(I_3^2-I_2^2)[I_2^2-(\mathcal{L}-\mathcal{L})^2]\cos 2\phi_2\big), \tag{32}$$

whereas the second contribution is a correction due to the coupling term

$$\frac{2}{\mathcal{H}'_{\mathrm{eff}_{00}}}\sum_{k\neq 0}\{\cdots\}=\frac{9}{20}\frac{\beta^2e}{\gamma M^2}\frac{1}{\mu^2k^2}\frac{I_3^2}{I_2^2}\Bigg[(-20(\mathcal{L}-\overline{\mathcal{L}})\times\left(\frac{p_1}{e}-\frac{Q}{e}(\mathcal{L}+\overline{\mathcal{L}})\right)I_2^2+5\frac{Q}{e}(I_3^2-I_2^2)\times[I_2^2+(\mathcal{L}-\overline{\mathcal{L}})^2]+5\frac{Q}{e}(I_3^2-I_2^2)\times[I_2^2-(\mathcal{L}-\overline{\mathcal{L}})^2]\cos 2\phi_2\Bigg]. \tag{33}$$

Scaling back to real time we, therefore, arrive at the final coupled equations of motion

$$\frac{dI_2}{d\mathcal{T}}=-\sigma^2\frac{\partial}{\partial\phi_2}\mathcal{H}_{\mathrm{eff}_{\mathrm{eff}}}(\sigma;I_2,\phi_2),$$
$$\frac{d\phi_2}{d\mathcal{T}}=\sigma^2\frac{\partial}{\partial I_2}\mathcal{H}_{\mathrm{eff}_{\mathrm{eff}}}(\sigma;I_2,\phi_2). \tag{34}$$

Let us now discuss the above results of the second averaging process. The averaged variable $\mathcal{L}$ is up to order $r=4$ an *approximate constant of motion*. By the second averaging of the equations of motion we have reduced the number of coupled degrees of freedom in fourth order from two to one. This means that our twice averaged system is integrable. It is a surprising result that the two contributions Eqs. (32) and (33) to the effective Hamiltonian Eq. (31) have, to some extent, a similar structure. Both the term arising from diamagnetism [Eq. (32)] as well as the term due to the coupling of the CM and relative motion [Eq. (33)] contain a $\cos 2\phi_2$ dependence on ϕ_2 and a prefactor involving a second-order polynomial in I_2^2. The first term in Eq. (33) represents, however, a qualitative difference between the two contributions (the case $M\to\infty$ which means, in particular, the absence of the contribution (33) has been treated in Ref. [16]). For an atomic system like the He^+ ion the ratio of the prefactors of the two contributions is $\delta\approx 72\mu^2/5M^2$ which shows the suppression of the contribution due to the coupling term for this extreme mass ratio.

In the following we discuss the solutions of the equations of motion (34). These solutions are periodic functions of time and will, together with their period, be given below as functions of the initial conditions. In order to integrate the equations of motion (34) we will take advantage of the conservation of $\mathcal{H}_{\mathrm{eff}_{\mathrm{eff}}}$. As a first step we define $\sigma^2\mathcal{H}_{\mathrm{eff}_{\mathrm{eff}}}:=\nu E$ with $\nu=\sigma^4\lambda/4\mu^2k^2I_3^4$. This gives us the angle ϕ_2 as a function of I_2 and the conserved momenta

$$\cos 2\phi_2=\frac{a(I_2/I_3)^4+b(I_2/I_3)^2+c}{d(I_2/I_3)^4+e(I_2/I_3)^2+f}, \tag{35}$$

with

$$a=\left(3+5\delta\frac{Q}{e}\right),$$
$$b=-5\left(1+\delta\frac{Q}{e}\right)+\left(3+5\delta\frac{Q}{e}\right)\frac{(\mathcal{L}-\overline{\mathcal{L}})^2}{I_3^2}+20\delta\frac{\mathcal{L}-\overline{\mathcal{L}}}{I_3^2}\times\left(\frac{p_1}{e}-\frac{Q}{e}(\mathcal{L}+\overline{\mathcal{L}})\right)+E=:b'+E,$$
$$c=-5\left(1+\delta\frac{Q}{e}\right)\frac{(\mathcal{L}-\overline{\mathcal{L}})^2}{I_3^2},$$
$$d=-5\left(1+\delta\frac{Q}{e}\right) \tag{36}$$

and $e=-c-d$, $f=c$. In the following we restrict ourselves to the physically interesting case $|\delta Q/e|<\frac{3}{5}$ which implies $a>0$, $c<0$, $d<0$, $d^2>a^2$. The curves $I_2(\phi_2)$ for constant energy possess the period π and are symmetric with respect to $\phi_2=n\,\pi/2$. E and b possess an absolute minimum at $\phi_2^{\min}=\pi/2$ and $I_2^{\min}=(2c/a+d)^{1/4}I_3$ and we have $b_{\min}=-2\sqrt{2c(a+d)}+c+d$. There exist two classes of curves. Librators are closed curves which exist in the vicinity of the above given minimum and are separated by a separatrix from the rotators which experience the whole range of possible values for ϕ_2. The separatrix is given by $b_{\mathrm{crit}}=-a-c$. For $2c>a+d$ both classes coexist whereas for $2c<a+d$ only rotators are present.

Using Eqs. (35) we can eliminate the angle ϕ_2 and obtain an ordinary differential equation for $I_2(\mathcal{T})$:

$$\frac{dI_2}{d\mathcal{T}} = -\frac{2\nu}{(I_2/I_3)^2} \pm \sqrt{[d(I_2/I_3)^4 + e(I_2/I_3)^2 + c]^2 - [a(I_2/I_3)^4 + b(I_2/I_3)^2 + c]^2}. \tag{37}$$

In order to integrate the above equation we have to establish the roots of the polynomial under the square root

$$P_1 = \frac{-b-c-d}{a-d},$$

$$P_2 = \frac{\sqrt{(e+b)^2 - 8c(d+a)} + (e+b)}{-2(a+d)},$$

$$P_3 = \frac{-\sqrt{(e+b)^2 - 8c(d+a)} + (e+b)}{-2(a+d)}, \tag{38}$$

which yields

$$d\mathcal{T} = -\frac{I_3}{4\nu} \frac{\pm}{\sqrt{d^2-a^2}} \frac{dP}{\sqrt{(P-P_1)(P-P_2)(P-P_3)}}. \tag{39}$$

P_3 is always the smallest root and belongs to the lower turning point at $\phi_2 = \pi/2$. P_1 and P_2 belong to the upper turning points of the librators and rotators, respectively. Due to the periodicity as well as the symmetry properties we have to integrate Eq. (39) only for the first half of the period of motion. The period finally can be obtained as

$$\mathcal{T}^{\phi_2} = \frac{I_3}{2\nu} \frac{1}{\sqrt{d^2-a^2}} \frac{2}{\sqrt{\max(P_1,P_2) - P_3}} \times F\left(\pi/2, \sqrt{\frac{\min(P_1,P_2)-P_3}{\max(P_1,P_2)-P_3}}\right), \tag{40}$$

where $F(\phi,k)$ is the elliptical function of the first kind [23]. The period $\mathcal{T}^{\phi_2}$ depends strongly on the values of the roots P_i, i.e., the initial conditions. On the separatrix $b = b_{\rm crit}\mathcal{T}^{\phi_2}$ diverges. The period $\mathcal{T}^{\phi_2}$ possesses however a lower bound

$$\mathcal{T}^{\phi_2} \geq T_d^{\phi_2 \min} := \frac{I_3}{\nu} \frac{\pi}{2\sqrt{2d(d-a)}}, \tag{41}$$

which can be considered a new third time scale which adds to the two previously discussed ones τ_K and $\overline{\tau}$.

For a discussion of the behavior of the decoupled coordinates (ξ, ϕ_3, ξ) belonging to the conserved momenta $(\mathcal{L}, I_3, \mathcal{L})$ we refer the reader to Ref. [22]. We remark here only that their typical time scales $\mathcal{T}^{\xi}, \mathcal{T}^{\phi_3}, \mathcal{T}^{\xi}$ are comparable to $\mathcal{T}^{\phi_2}$ and these four quantities therefore define one common time scale of the doubly averaged motion.

In the remaining part of the paper we report on the interpretation of the above obtained results in Cartesian coordinates and build a bridge to the numerically observed phenomena in Ref. [74]. In order to get the time-dependent dynamics of the Cartesian CM coordinates and velocities we exploit Eqs. (A4)–(B5) and use the relation

$$\dot{\mathbf{R}}_{\rm cm} = \frac{1}{M} \mathbf{\Pi}_{\rm cm} - \frac{\beta}{M} \mathbf{B} \times \mathbf{r},$$

where $\Pi_{\rm cm}$ is given in Eq. (A1). First of all we emphasize that all numerically observed time scales of the motion of the CM can be found and are described in detail by our perturbation theoretical approach. The individual oscillations on the shortest time scale τ_K can be obtained by the unaveraged Hamiltonian equations of motion. The modulations of the CM energy on the time scale $\overline{\tau}$ are precisely described by the once averaged perturbation theoretical equations. The dynamical behavior for times $t \geq \overline{\tau}$ is best described by the twice averaged equations of motion and gives the additional modulations of the CM motion on the typical time scale $\mathcal{T}^{\phi_2}$.

Finally on the largest time scale τ_Z the CM motion closes to a circular orbit with radius

$$R_Z = \left| \frac{M}{QB^2} \mathbf{B} \times \dot{\mathbf{R}}_{\rm cm}(0) - \frac{\beta}{Q} \mathbf{r}_\perp(0) \right|. \tag{42}$$

and cyclotron frequency $\omega_Z := \gamma_Z \sigma^2$. Equation (42) now establishes the self-stabilization effect in a rigorous analytical way. In particular, it demonstrates that the CM of the ion stabilizes for vanishing initial CM velocity on a cyclotron orbit whose radius is, apart from constant factors, determined by the initial relative distance of the two particles perpendicular to the magnetic field. We conclude with the remark that this effect is ultimately a consequence of the action of the coupling Hamiltonian $H^{[2]}$, H_3.

V. SUMMARY AND CONCLUSIONS

We have investigated the classical dynamics and properties of charged two-body systems in a magnetic field in the regular, i.e., by perturbation-theory accessible, regime. This system possesses three exact commuting constants of motion: the component of the total momentum parallel to the field, the corresponding component of the total angular momentum as well as the square of the absolute value of the pseudomomentum perpendicular to the magnetic field. In a first step these conserved quantities have been introduced by a number of subsequent canonical transformations as canonical momenta, thereby eliminating their cyclic coordinates. At the same time we introduced a field-dependent scale transformation which brings the Hamiltonian to a form well suited for the application of perturbation theory. In particular, the coupling term between the CM and relative motion is in this representation proportional to a single low power of the field strength. By the above canonical transformations the number of coupled degrees of freedom was reduced from six to three which means a five-dimensional energy shell in phase space.

Next we applied two perturbation theoretical concepts to the resulting exact Hamiltonian equations of motion: a perturbation theoretical series expansion due to the explicit as well as implicit dependence of the equations on the parameter $\sigma:=B^{1/2}$ and a time averaging procedure. Both approaches are in some detail described in Appendix C of the present work. The latter perturbation theoretical concept was motivated by the fact that the system under consideration possesses several by orders-of-magnitude different time scales which manifest themselves in the perturbation theoretical equations of motion. The series expansion by itself allows only for a determination of the short-time dynamics whereas the long-time behavior is accessible by the averaged equations of motion. Our first application of the averaging procedure revealed already interesting properties: the principal action of the Kepler problem proved to be a constant of motion up to fourth order in perturbation theory. The number of coupled degrees of freedom, therefore, reduced from three to two after the first averaging. An effective Hamiltonian which describes the averaged dynamics for the two remaining degrees of freedom could be presented.

After another field-dependent scale transformation a second averaging process could be performed which finally renders the system integrable. The canonical momentum $\mathcal{L}$ turns out to be an additional constant of motion up to fourth-order perturbation theory. $\mathcal{L}$ is the difference between the angular momentum components of the CM and relative motion. Since the total angular momentum component $\mathcal{L}$ is exactly conserved this means, that, on the level of the twice averaged equations of motion, the coupling between the CM and relative motion causes in fourth-order perturbation theory only an exchange of energy but no exchange of angular momentum components parallel to the field. The number of coupled degrees of freedom is now reduced from two to one and we encounter on this large time scale an integrable averaged motion described by an effective Hamiltonian $\mathcal{H}_{\mathrm{eff}_{\mathrm{eff}}}$. The solutions as well as phase-space structure of this Hamiltonian are calculated and discussed in detail. The existence of rotating and librating trajectories is established and their periods are given analytically as a function of the initial conditions.

The above procedure provides an analytical manifestation of the existence of four different time scales of the CM motion of the ion which have very recently been observed in numerical simulations [14]. Apart from this it provides, in addition, an analytical approach to the classical self-stabilization effect of the ion. The radius as well as the frequency of the cyclotron orbit of the CM motion with initially vanishing CM velocity can be calculated explicitly and the self-stabilization effect can, therefore, be understood in the general framework of the phenomena arising in the regular regime.

One of the authors (P.S.) acknowledges financial support by the Deutsche Forschungsgemeinschaft.

APPENDIX A: THE CANONICAL CENTER OF MASS VARIABLES

Let us introduce the kinetic as well as pseudomomentum of the CM

$$\mathbf{\Pi}_{\mathrm{cm}}=\mathbf{P}_{\mathrm{cm}}-\frac{Q}{2}\,\mathbf{B}\times\mathbf{R}_{\mathrm{cm}},$$

$$\mathbf{K}_{\mathrm{cm}}=\mathbf{P}_{\mathrm{cm}}+\frac{Q}{2}\,\mathbf{B}\times\mathbf{R}_{\mathrm{cm}}, \tag{A1}$$

which are related to the angular momentum of the CM in the following way:

$$2QBL_{\mathrm{cm}z}=\mathbf{K}_{\mathrm{cm}\perp}^2-\mathbf{\Pi}_{\mathrm{cm}\perp}^2. \tag{A2}$$

Choosing the set $(p_1,p_2,p_3)=(\mathbf{K}_{\mathrm{cm}\perp}^2/2B,L_{\mathrm{cm}z},P_{\mathrm{cm}z})$ as canonical momenta it is possible to derive the following transformation formulas:

$$p_1=\frac{\mathbf{K}_{\mathrm{cm}\perp}^2}{2B};\quad \cos Qq_1=\frac{\mathbf{K}_{\mathrm{cm}\perp}\mathbf{\Pi}_{\mathrm{cm}\perp}}{|\mathbf{K}_{\mathrm{cm}\perp}||\mathbf{\Pi}_{\mathrm{cm}\perp}|};$$

$$\sin Qq_1=\frac{(\mathbf{K}_{\mathrm{cm}\perp}\times\mathbf{\Pi}_{\mathrm{cm}\perp})_z}{|\mathbf{K}_{\mathrm{cm}\perp}||\mathbf{\Pi}_{\mathrm{cm}\perp}|},$$

$$p_2=L_{\mathrm{cm}z};\quad \cos q_2=\frac{\Pi_{\mathrm{cm}\,x}}{|\mathbf{\Pi}_{\mathrm{cm}\perp}|};\quad \sin q_2=\frac{\Pi_{\mathrm{cm}\,y}}{|\mathbf{\Pi}_{\mathrm{cm}\perp}|},$$

$$p_3=P_{\mathrm{cm}z};\quad q_3=Z_{\mathrm{cm}} \tag{A3}$$

With some calculation we arrive at the inverse transformation laws

$$X_{\mathrm{cm}}=\frac{1}{QB}\left[\sqrt{2Bp_1}\sin(Qq_1+q_2)-\sqrt{2B(p_1-Qp_2)}\,\sin q_2\right],$$

$$Y_{\mathrm{cm}}=-\frac{1}{QB}\left[\sqrt{2Bp_1}\cos(Qq_1+q_2)\right.$$
$$\left.-\sqrt{2B(p_1-Qp_2)}\cos q_2\right],$$

$$Z_{\mathrm{cm}}=q_3,$$

$$P_{\mathrm{cm}x}=\tfrac{1}{2}\left[\sqrt{2Bp_1}\cos(Qq_1+q_2)+\sqrt{2B(p_1-Qp_2)}\cos q_2\right],$$

$$P_{\mathrm{cm}y}=\tfrac{1}{2}\left[\sqrt{2Bp_1}\sin(Qq_1+q_2)+\sqrt{2B(p_1-Qp_2)}\sin q_2\right],$$

$$P_{\mathrm{cm}z}=p_3, \tag{A4}$$

APPENDIX B: THE ACTION-ANGLE VARIABLES OF THE KEPLER PROBLEM

For the details of the derivation of the action-angle variables for the Kepler problem we refer the reader to the literature [16,21]. In the following we provide only some of the key relationships among the different relevant quantities. We define the action variables

$$I_1=l_z,$$

$$I_2=l,$$

$$I_3=\left(\frac{\mu k^2}{-2H}\right)^{1/2}, \tag{B1}$$

where L is the absolute value of the total canonical angular momentum and H the Kepler-Hamiltonian. In addition we introduce the true anomaly χ, the eccentric anomaly ψ, as well as the mean anomaly, which is the canonical angle ϕ_3. These quantities are related by the following equations:

$$\phi_3 = \psi - \varepsilon \sin\psi,$$

$$\tan\frac{\chi}{2} = \left(\frac{1+\varepsilon}{1-\varepsilon}\right)^{1/2} \tan\frac{\psi}{2}, \tag{B2}$$

where

$$\varepsilon(I_2, I_3) = \left(1 - \frac{I_2^2}{I_3^2}\right)^{1/2} \tag{B3}$$

is the eccentricity of the ellipse. From the focal representation of the ellipse we obtain for the radius

$$r = \frac{I_2^2 mk}{1 + \varepsilon(I_2, I_3)\cos\chi(I_2, I_3, \phi_3)}, \tag{B4}$$

where the true anomaly is given in Eqs. (B2). The radius vector reads as follows:

$$\mathbf{r}(I_1, I_2, I_3, \phi_2, \phi_3) = r(I_2, I_3, \phi_3) \begin{pmatrix} \cos\phi_1 \cos(\phi_2+\chi) - \sin\phi_1 \sin(\phi_2+\chi)\, \dfrac{I_1}{I_2} \\ \sin\phi_1 \cos(\phi_2+\chi) + \cos\phi_1 \sin(\phi_2+\chi)\, \dfrac{I_1}{I_2} \\ \sin(\phi_2+\chi)\left(1 - \dfrac{I_1^2}{I_2^2}\right)^{1/2} \end{pmatrix} \tag{B5}$$

APPENDIX C: THE PERTURBATION THEORETICAL METHOD

Our starting situation possesses the following characteristics: The underlying exact Hamiltonian can be represented in a series, in our case up to fourth order, in a small parameter σ; in the lowest order σ^0 only a single variable, namely, ϕ_3, is not constant; the total Hamiltonian is a periodic function of this variable [see Eqs. (16)–(20)]. The aim of the present appendix is to derive the perturbation theoretical Hamiltonian equations of motion which have been averaged over one time cycle of the distinguished variable ϕ_3. Our method can be applied to any problem meeting the above characteristics and is therefore by no means restricted to the case of interest of the present paper, i.e., highly excited charged two-body systems in a magnetic field. The above conditions are not as special as they might seem from a first glance. Indeed, if possible one would always choose as a zeroth-order Hamiltonian an integrable one which meets in suitable action-angle variables the first two of the above conditions.

Let us begin with a perturbation theoretical expansion of the Hamiltonian and its equations of motion according to the explicit as well as implicit dependence on the small parameter σ. According to our assumption the explicit dependence of the Hamiltonian on the parameter σ can be represented in a series

$$H(\sigma;\mathbf{p},\mathbf{q}) = \sum_{l=0}^{\infty} \sigma^l / l!\, H_l(\mathbf{p},\mathbf{q}), \tag{C1}$$

Of course, the solutions, i.e., coordinates and momenta $q(\sigma;t)$ and $p(\sigma;t)$, depend implicitly on the parameter σ which can also be expanded in a series

$$p_i(\sigma;t) = \sum_{r=0}^{\infty} \sigma^r / r!\, p_{ir}(t) \quad \text{with} \quad p_{ir}(t) := \frac{\partial^r}{\partial\sigma^r}\, p_i(\sigma;t),$$

$$q_i(\sigma;t) = \sum_{r=0}^{\infty} \sigma^r / r!\, q_{ir}(t) \quad \text{with} \quad q_{ir}(t) := \frac{\partial^r}{\partial\sigma^r}\, q_i(\sigma;t). \tag{C2}$$

These expansions possess only a finite radius of convergence. To get the long-time behavior we will in general have to apply the time-averaging procedure described below. The total expansion of the Hamiltonian with respect to the parameter σ can after some calculation be obtained as

$$H[\sigma;\mathbf{p}(\sigma),\mathbf{q}(\sigma)]$$

$$= \sum_{r=0}^{\infty} \sigma^r / r!\, H^{(r)}(\mathbf{p}_0, \mathbf{q}_0 | \mathbf{p}_1, \ldots, \mathbf{p}_r, \mathbf{q}_1, \ldots, \mathbf{q}_r), \tag{C3}$$

where $H^{(r)}$ is defined as

$$H^{(r)}(\mathbf{p}_0, \mathbf{q}_0 | \mathbf{p}_1, \ldots, \mathbf{p}_r, \mathbf{q}_1, \ldots, \mathbf{q}_r)$$

$$= \sum_{l+s=n} \binom{r}{s} \sum^{(s)} (\mathbf{p}_1, \ldots, \mathbf{p}_s, \mathbf{q}_1, \ldots, \mathbf{q}_s) H_l(\mathbf{p}_0, \mathbf{q}_0), \tag{C4}$$

with

$$\sum^{(s)}(\mathbf{p}_1,\ldots,\mathbf{p}_s,\mathbf{q}_1,\ldots,\mathbf{q}_s)=\begin{cases}1; & s=0\\ \sum_{\nu=1}^{s}1/\nu!\sum_{\substack{r_\alpha\geqslant 1\\ r_1+\cdots+r_\nu=s}}\left\{\frac{s!}{r_1!\ldots r_\nu!}D_{r_1}(\mathbf{p}_{r_1},\mathbf{q}_{r_1})\ldots\ldots D_{r_2}(\mathbf{p}_{r_\nu},\mathbf{q}_{r_\nu})\right\}; & s\neq 0\end{cases}\tag{C5}$$

and for $r\geqslant 1$

$$D_r(\mathbf{p}_r,\mathbf{q}_r)=\left(p_{ir}\frac{\partial}{\partial p_{i0}}+q_{ir}\frac{\partial}{\partial q_{i0}}\right).\tag{C6}$$

The Hamiltonian equations of motion for each order read as follows:

$$\dot{p}_{ir}=-\frac{\partial}{\partial q_{i0}}H^{(r)}(\mathbf{p}_0,\mathbf{q}_0|\mathbf{p}_1,\ldots,\mathbf{p}_r,\mathbf{q}_1,\ldots\mathbf{q}_r),$$

$$\dot{q}_{ir}=\frac{\partial}{\partial p_{i0}}H^{(r)}(\mathbf{p}_0,\mathbf{q}_0|\mathbf{p}_1,\ldots,\mathbf{p}_r,\mathbf{q}_1,\ldots,\mathbf{q}_r),\tag{C7}$$

which shows that $H^{(r)}$ alone determines the rth order of p and q. The dynamics of the variables in rth order depend therefore on all variables of orders $\leqslant r$. Since the equation of motion for the rth order of a certain variable depends not only on the lower orders but also on the rth order of the other variables it is in general not obvious how Eqs. (C7) could be solved. However, Eqs. (C7) are very helpful and much easier to solve than the exact equations of motion if the zeroth-order Hamiltonian has a particularly simple structure and depends only on a few variables which is definitely the case for our chosen Hamiltonian (see comments at the beginning of this appendix). This becomes particularly obvious if we decompose

$$\begin{aligned}H^{(r)}&(\mathbf{p}_0,\mathbf{q}_0|\mathbf{p}_1,\ldots,\mathbf{p}_r,\mathbf{q}_1,\ldots,\mathbf{q}_r)\\&=\widetilde{H}^{(r)}(\mathbf{p}_0,\mathbf{q}_0|\mathbf{p}_1,\ldots,\mathbf{p}_{r-1},\mathbf{q}_1,\ldots,\mathbf{q}_{r-1})\\&\quad+\sum^{(r)}(\mathbf{p}_1,\ldots,\mathbf{p}_r,\mathbf{q}_1,\ldots,\mathbf{q}_r)H_0(\mathbf{p}_0,\mathbf{q}_0)\end{aligned}\tag{C8}$$

according to which the part of rth order appears only in connection with the Hamiltonian of zeroth order and any simplification of the zeroth-order Hamiltonian therefore results in a major simplification of the Hamiltonian equations of motion of rth order. Similarly simplifications of the higher orders H_l of the Hamiltonian will also lead to simplifications of the Hamiltonian equations of motion of orders $r\geqslant l$.

As already mentioned we deal in our particular case with an integrable Hamiltonian H_0 which depends on only one canonical momentum p_1, i.e., we have $H_0(\mathbf{p},\mathbf{q})=h(p_1)$. Using this fact Eqs. (C7) take on the following appearance:

$$\dot{p}_{ir}=-\frac{\partial}{\partial q_{i0}}\widetilde{H}^{(r)}(\mathbf{p}_0,\mathbf{q}_0|\mathbf{p}_1,\ldots,\mathbf{p}_{r-1},\mathbf{q}_1,\ldots,\mathbf{q}_{r-1}),\tag{C9}$$

$$\begin{aligned}\dot{q}_{1r}=&\frac{\partial}{\partial p_{10}}\widetilde{H}^{(r)}(\mathbf{p}_0,\mathbf{q}_0|\mathbf{p}_1,\ldots,\mathbf{p}_{r-1},\mathbf{q}_1,\ldots,\mathbf{q}_{r-1})\\&+\Upsilon^{(r)}(p_{11},\ldots,p_{1r})\frac{\partial}{\partial p_{10}}h(p_{10}),\end{aligned}\tag{C10}$$

$$\dot{q}_{ir}=\frac{\partial}{\partial p_{i0}}\widetilde{H}^{(r)}(\mathbf{p}_0,\mathbf{q}_0|\mathbf{p}_1,\ldots,\mathbf{p}_{r-1},\mathbf{q}_1,\ldots,\mathbf{q}_{r-1}),\quad i\neq 1.\tag{C11}$$

Apart from the second term on the right-hand side of Eqs. (C10), the above equations of motion of order r involve only quantities of order $r-1$ and are therefore almost decoupled. The remaining coupling term reads as follows:

$$\begin{aligned}\Upsilon^{(r)}(p_{11},\ldots,p_{1r})h(p_{10}):=&\sum^{(r)}(\mathbf{p}_1,\ldots,\mathbf{p}_r,\mathbf{q}_1,\ldots,\mathbf{q}_r)\\&\times H_0(\mathbf{p}_0,\mathbf{q}_0).\end{aligned}\tag{C12}$$

Due to the simple structure of the equations of motion (C9)–(C11) the solution of order r can be obtained from the solutions of order $r-1$ in the following way. First we obtain by ordinary time integrations $p_{ir}(t),q_{ir}(t)$ except $q_{1r}(t)$ from Eqs. (C9)–(C11). Inserting these solutions into Eq. (C10) yields again by ordinary time integration also $q_{1r}(t)$. The equations of motion can therefore be solved to any order iteratively by ordinary time integrations. This should not obscur the fact that our expansion possesses a finite radius of convergence $\sigma_f(t)>0$ for $t<t_f$, i.e., converges only for a certain propagation time of the trajectory. However, the above choice enhances the chance of good convergence properties, since only one variable (ϕ_3) occupies in zeroth order an unbounded coordinate range.

To get the classical behavior on a long time scale we will apply in addition to the above discussed perturbation theory a time-averaging procedure whose fundamental equations and properties will be derived in the remaining part of this appendix. By performing a time-averaging procedure we are no more interested in the fine structure of the dynamics of our system but in its averaged behavior. The averaging-time scale can, for example, be the shortest time scale associated with the time dependence of the coordinate q_1. Following this way we will obtain effective equations of motion which describe the deviation of the real motion from the fast oscillatory motion.

The first step is to divide the time axis in intervals $I(n)$ so that the length $\Delta T(n)$ of each interval is less than t_f. Instead of the original initial value problem we consider the initial value problem for each interval separately, perform the averaging procedure, and will finally link them in a well-defined way together (see below). The equations describing the changes $\Delta p(n),\Delta q(n)$ during the nth averaging period depend on the corresponding initial values $p(n),q(n)$ and represent a system of difference equations in n which can be determined to some desired order r in the perturbation parameter σ. The lengths of the averaging periods $\Delta T(n)$ can now be chosen in such a way that the resulting equations take on a particularly simple form. We hereby take advantage of the fact that the only dynamic variable in zeroth order is q_1 and that the exact Hamiltonian is periodic in q_1 with period 2π. The optimal choice is therefore $\Delta T(n)=2\pi/h'(p_1(n))$ which takes into account that the time intervals of averaging have to be adapted to the momentary values of the momentum p_1. The time-averaging interval depends therefore on the step n and has to be calculated together with the changes in the coordinates and momenta.

In order to perform the averaging we represent all periodic functions in Fourier series

$$H_l(\mathbf{p},\mathbf{q})=\sum_{k=-\infty}^{\infty} H_{lk}(\mathbf{p},q_2,\ldots,q_m)e^{ikq_1}. \tag{C13}$$

Having done this we are now in a position to express the initial value problem of the changes of the variables during one cycle to arbitrary order in the parameter σ as a series of elementary integrals. Subsequently performing these integrals we obtain difference equations of the following appearance:

$$\frac{\Delta\mathbf{p}(\sigma;n)}{\Delta T(n)}=f(\sigma;\mathbf{p}(n),\mathbf{q}(n))$$

$$\frac{\Delta\mathbf{q}(\sigma;n)}{\Delta T(n)}=g(\sigma;\mathbf{p}(n),\mathbf{q}(n)) \tag{C14}$$

which go up to a certain desired order in their explicit dependence on the parameter σ. However, the functions f,g depend also implicitly via the initial values $p(n),q(n)$ on any order of σ. To obtain the final working difference equations one has to perform the expansion with respect to the explicit as well as implicit dependence of the functions f,g on the parameter σ. How this has to be done was described in the first part of this appendix, now with the minor difference that we are dealing with difference equations instead of differential equations and with the fact that f,g can not necessarily be obtained as partial derivatives of a single function, i.e., the equations do not necessarily possess Hamiltonian structure (see below). The resulting system of difference equations in some pure order of σ are finally replaced by differential equations which describe the smooth behavior of the averaged variables and take on the following structure:

$$\frac{d\mathbf{p}_r(T)}{dT}=f^{(r)}(\mathbf{p}_0(T),\mathbf{q}_0(T)|\mathbf{p}_1(T),\ldots,\mathbf{p}_r(T),\mathbf{q}_1(T),\ldots,\mathbf{q}_r(T)),$$

$$\frac{d\mathbf{q}_r(T)}{dT}=g^{(r)}(\mathbf{p}_0(T),\mathbf{q}_0(T)|\mathbf{p}_1(T),\ldots,\mathbf{p}_r(T),\mathbf{q}_1(T),\ldots,\mathbf{q}_r(T)), \tag{C15}$$

where we have used T to describe the continuous time dependence of the averaged variables. The property that the zeroth-order Hamiltonian depends only on p_1 translates now into the fact that only $g_1(0)$ is nonzero for $r=0$. We give the zeroth and first-order equations explicitly

$r=0$:

$$f_i^{(0)}(\mathbf{p}_0(T),\mathbf{q}_0(T))=0,$$

$$g_1^{(0)}(\mathbf{p}_0(T),\mathbf{q}_0(T))=h'(p_{10}(T))$$

$$g_i^{(0)}(\mathbf{p}_0(T),\mathbf{q}_0(T))=0;\quad i\neq 1 \tag{C16}$$

$r=1$:

$$f_1^{(1)}(\mathbf{p}_0(T),\mathbf{q}_0(T)|\mathbf{p}_1(T),\mathbf{q}_1(T))=0,$$

$$f_i^{(1)}(\mathbf{p}_0(T),\mathbf{q}_0(T)|\mathbf{p}_1(T),\mathbf{q}_1(T)) =-\frac{\partial H_{10}}{\partial q_{i0}(T)}(\mathbf{p}_0(T),q_{20}(T),\ldots,q_{n0}(T));\quad i\neq 1,$$

$$g_1^{(1)}(\mathbf{p}_0(T),\mathbf{q}_0(T)|\mathbf{p}_1(T),\mathbf{q}_1(T)) =\frac{\partial H_{10}}{\partial p_{10}(T)}(\mathbf{p}_0(T),q_{20}(T),\ldots,q_{n0}(T)) +\langle p_{11}\rangle_n(\mathbf{p}_0(T),\mathbf{q}_0(T))h''(p_{10}(T))+p_{11}(T)h''(p_{10}(T))$$

$$g_i^{(1)}(\mathbf{p}_0(T),\mathbf{q}_0(T)|\mathbf{p}_1(T),\mathbf{q}_1(T)) =\frac{\partial H_{10}}{\partial p_{i0}(T)}(\mathbf{p}_0(T),q_{20}(T),\ldots,q_{n0}(T));\quad i\neq 1. \tag{C17}$$

For the particular example of a charged two-body system in a magnetic field our perturbation theoretical averaged equations of motion show for the coupled variables up to fourth order in σ a Hamiltonian structure, i.e., they can be derived from an effective Hamiltonian H_{eff} (see Sec. IV). For further details on our perturbation theoretical approach we refer the reader to Ref. [22].

APPENDIX D: THE FOURIER COMPONENTS OF THE HAMILTONIAN

In this appendix we provide the Fourier components of the Hamiltonians needed in our perturbation theoretical calculation of Sec. IV. The Hamiltonian depends periodically on the variables ϕ_3 and ξ whose corresponding Fourier components are given in Secs. D 1 and D 2, respectively.

1. The periodicity in ϕ_3

The components H_l of the Hamiltonian (16) are periodic with respect to ϕ_3. Since the components of zeroth and second order do not depend on ϕ_3 at all their Fourier representation is trivial, i.e., we have

$$H_{0k}(p_3;I_3)=\begin{cases}H_0(p_3;I_3); & k=0\\ 0 & \text{else,}\end{cases} \tag{D1}$$

$$H_{2k}(\mathcal{L},p_1;\overline{\mathcal{L}})=\begin{cases}H_2(\mathcal{L},p_1;\overline{\mathcal{L}}); & k=0\\ 0 & \text{else.}\end{cases} \tag{D2}$$

Due to the averaging process we need from the third and fourth order Hamiltonian H_3 and H_4 only the zeroth Fourier components which can after some calculation be obtained as

$$H_{30}(\mathcal{L},p_1;I_3;\overline{\mathcal{L}},I_2,\overline{\xi},\phi_2)=9\frac{\sqrt{2}\beta}{M}\sqrt{p_1-Q(\mathcal{L}+\mathcal{L})}\,\frac{I_3}{\mu k}\times\sqrt{I_3^2-I_2^2}\left(\sin\overline{\xi}\cos\phi_2-\cos\overline{\xi}\sin\phi_2\frac{\mathcal{L}-\overline{\mathcal{L}}}{I_2}\right), \tag{D3}$$

and

$$H_{40}(\mathcal{L};I_3;\overline{\mathcal{L}},I_2,\phi_2)=\frac{6\lambda}{\mu^2k^2}\frac{I_3^2}{I_2^2}\big((5I_3^2-3I_2^2)[I_2^2+(\mathcal{L}-\overline{\mathcal{L}})^2]+5(I_3^2-I_2^2)[I_2^2-(\mathcal{L}-\overline{\mathcal{L}})^2]\cos2\phi_2\big). \tag{D4}$$

2. The periodicity in $\overline{\xi}$

The Hamiltonian (16) is also periodic with respect to $\overline{\xi}$. However, we do not need the Fourier components of this original Hamiltonian but of the averaged Hamiltonian H_{eff} in Eq. (29). According to Sec. IV and Appendix C we need now not only the zeroth but all Fourier components. We obtain after some calculation

$$H_{\mathrm{eff}_{0k}}(\mathcal{L},p_1;\overline{\mathcal{L}})=\begin{cases}H_{\mathrm{eff}_{0k}}(\mathcal{L},p_1;\overline{\mathcal{L}})=\overline{\gamma\overline{\mathcal{L}}}+\gamma\mathcal{L}+\dfrac{p_1}{M}; & k=0\\ 0 & \text{else,}\end{cases} \tag{D5}$$

$$H_{\mathrm{eff}_{2k}}(\mathcal{L};I_3;\overline{\mathcal{L}},I_2,\phi_2)=\begin{cases}H_{\mathrm{eff}_2}(\mathcal{L};I_3;\overline{\mathcal{L}},I_2,\phi_2)=\frac{1}{12}H_{40}(\mathcal{L};I_3;\overline{\mathcal{L}},I_2,\phi_2); & k=0\\ 0 & \text{else.}\end{cases} \tag{D6}$$

The only nonvanishing Fourier components for the Hamiltonian H_{eff_1} are those with $k=1,-1$. It can be shown that

$$H_{\mathrm{eff}_{11}}(\overline{\mathcal{L}},I_2,I_3,\phi_2)=-\frac{3}{4}\frac{\sqrt{2}\beta}{M}\sqrt{p_1-Q(\mathcal{L}+\mathcal{L})}\,\frac{I_3}{\mu k}\sqrt{I_3^2-I_2^2}\left(\sin\phi_2\frac{\mathcal{L}-\overline{\mathcal{L}}}{I_2}+i\cos\phi_2\right),$$

$$H_{\mathrm{eff}_{1(-1)}}=H^*_{\mathrm{eff}_{11}}$$

$$H_{\mathrm{eff}_{1k}}=0;\quad k\notin\{-1,1\}, \tag{D7}$$

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