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# Saddle-node bifurcation for Rydberg atoms in parallel electric and magnetic fields

J. P. Salas
*Area de Física Aplicada, Universidad de La Rioja, 26004 Logroño, Spain*

V. Lanchares
*Departamento de Matemáticas y Computación, Universidad de La Rioja, 26004 Logroño, Spain*

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A comprehensive study of the hydrogen atom in the presence of parallel electric and magnetic fields is presented from the standpoint of classical mechanics for a nonzero magnetic quantum number $m$. The transition from pure Zeeman effect to Stark effect is explored intensively by means of Poincaré surfaces of section for a pair of $m$ values and for different values of the field strengths. It is found that the transition from pure Zeeman effect to Stark effect passes through a *saddle-node* bifurcation. [S1050-2947(98)01507-8]

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## I. INTRODUCTION

This paper is the third one of a series of articles that the authors dedicate to the classical study of the SQZE problem. The first one (Deprit *et al.* [1]) deals with the analytic study of the normalized problem when the magnetic quantum number $m$ is not zero using action angle variables closely related to those introduced in the treatment of the pure Zeeman effect [2–4]. In this perturbative model it is proven that the transition from the pure Zeeman to pure Stark effect passes through a *teardrop* bifurcation when $m$ is below the critical value $m_c = n/\sqrt{5}$. However, this result is obtained after averaging the results from asymptotic expansions and the convergence and the domain of validity are not discussed. Therefore, it was necessary to obtain the same results by means of different techniques in order to validate them.

The objective of this article is to state a classical description of the phase space (electronic) structure for Rydberg atoms in the presence of parallel electric and magnetic fields [the Stark quadratic Zeeman effect (SQZE) problem] when the magnetic quantum number $m$ is not zero by applying the method of the Poincaré surfaces of section [5].

In the second paper of the series (Salas *et al.* [6]), the problem is treated when the magnetic quantum number $m$ is zero, the so-called polar case. In this case, by means of perturbation methods and Poincaré surfaces of section, the evolution from the Zeeman to the Stark effect is explained as the result of two *pitchfork* bifurcations.

The literature on this subject is rather extensive, so much so that for a review we refer the reader to the theoretical works of Braun and Solove'v [7], Waterland *et al.* [8], Farrelly *et al.* [9], Braun [10], Deprit *et al.* [1], and Milczewski and Uzer [11], and to the experimental works of Cacciani *et al.* [12–14].

For the present nonpolar case ($m \neq 0$), we consider that, as in the previous works in the literature, the electric and magnetic interactions are weak compared to the Coulombian field. With this assumption, the system is very close to its integrable limit, which corresponds to the nonperturbed Rydberg atom. In this way, only the regular regime in the SQZE needs to be taken into account. This hypothesis will also allow us to compare the results here obtained with those obtained by means of the perturbative study of our first work [1].

The paper is organized as follows: in Sec. II the problem is briefly stated. In Sec. III, for a pair of $m$ values and for different values of the field strengths, we explore the evolution of the surfaces of section when the transition from the Zeeman to the Stark effect takes place. Special attention is paid to the stability of the fixed points appearing in the surfaces of section, in the bifurcations between them and in the relation with the experimental and theoretical investigations of Cacciani *et al.* [12–14]. In Sec. IV we relate the evolution of the dimensionless orbital elements of the periodic orbits appearing in the surfaces of section to the evolution of the dimensionless orbital elements of the equilibria of the normalized problem. Finally, Sec. V contains a short discussion about the results.

## II. PROBLEM

In cylindrical coordinates and atomic units, the hydrogen atom in the presence of parallel electric and magnetic fields is described by the two-dimensional Hamiltonian [9]

$$\mathcal{H} = E = \frac{1}{2}\left(P_\rho^2 + P_z^2 + \frac{m^2}{\rho^2}\right) - \frac{1}{\sqrt{\rho^2+z^2}} + \frac{\gamma^2}{8}\rho^2 + fz, \quad (1)$$

where $z$ is the coordinate parallel to the fields, $\gamma$ and $f$ are, respectively, the magnetic and electric field strengths and $m$ is the $z$ component of the angular momentum $\mathbf{L}$. We suppose $m$ to be nonzero. Now, according to [15], it is convenient to scale coordinates and momenta $\hat{\mathbf{r}} = \gamma^{2/3}\mathbf{r}$, $\hat{\mathbf{P}} = \gamma^{-1/3}\mathbf{P}$. After dropping hats in the coordinates and momenta, Hamiltonian (1) becomes

$$\hat{\mathcal{H}} = \mathcal{H}\gamma^{-2/3} = \epsilon = \frac{1}{2}\left(P_\rho^2 + P_z^2 + \frac{\hat{m}^2}{\rho^2}\right) - \frac{1}{\sqrt{\rho^2+z^2}} + \frac{1}{8}\rho^2 + \mathcal{F}z, \quad (2)$$

 

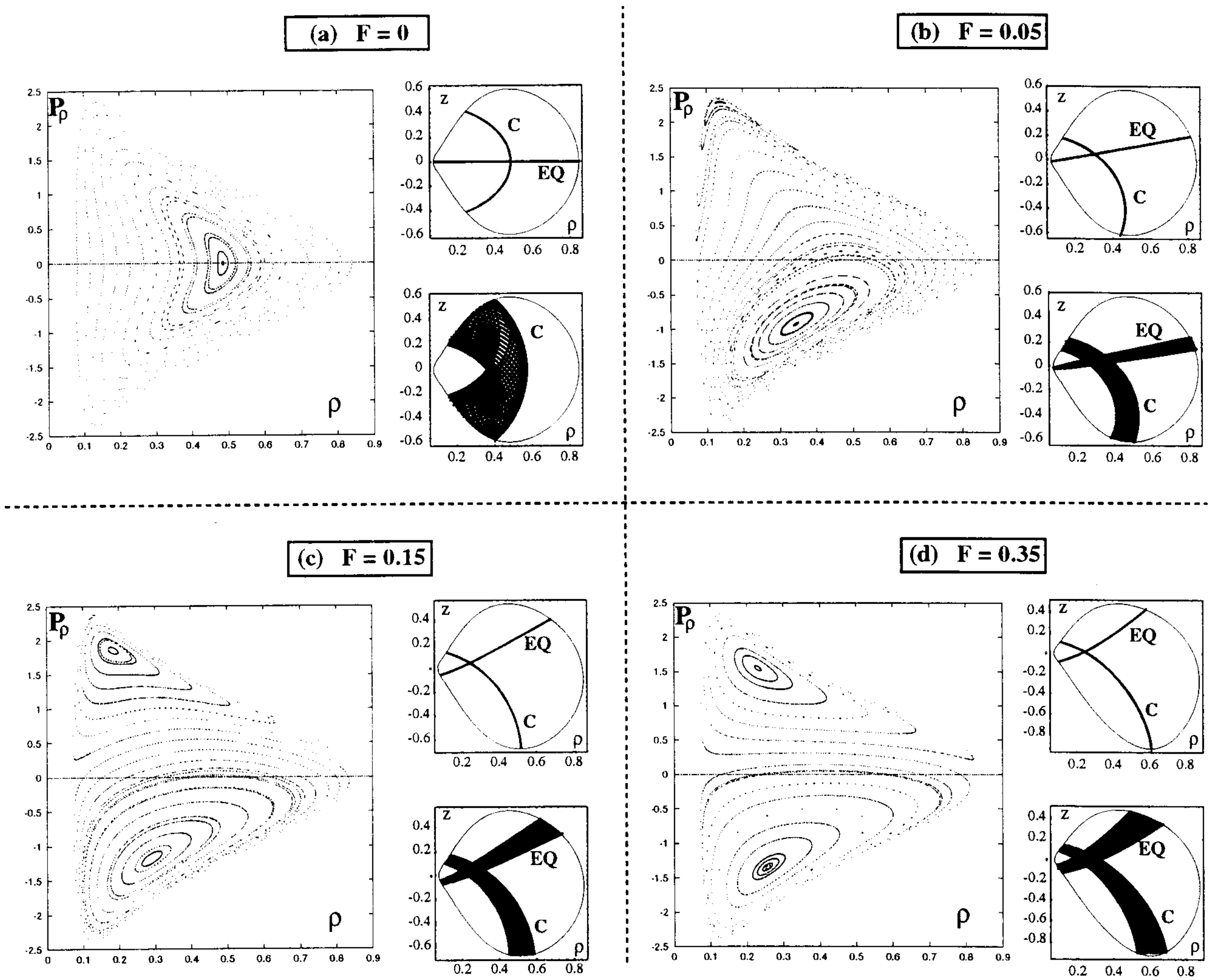


FIG. 1. Evolution of the Poincaré surfaces of section, periodic orbits, and quasiperiodic levels as a function of the parameter $\mathcal{F}$ for $m=0.28$ and $\epsilon=-1$.

and the classical dynamics depends only on the three scaled parameters $\epsilon=\gamma^{-2/3}E$, $\hat{m}=\gamma^{1/3}m$, and $\mathcal{F}=\gamma^{-4/3}f$. The parameter $\mathcal{F}$ represents the relative influence of the magnetic and the electric field strengths.

We use the Poincaré surfaces of section technique to formulate a description of the classical electronic structure of the problem: by keeping $\epsilon$ and $\hat{m}$ constant and by tuning the parameter $\mathcal{F}$, we can explore the structure of the surfaces of section as the system evolves from the pure Zeeman effect ($\mathcal{F}=0$) to the Stark effect. Moreover, we will show that the behavior described by means of surfaces of section coincides qualitatively with the behavior found by means of classical perturbation methods.

We define the surface of section as $z=0$, $P_z>0$. Under these conditions, the surface of section appears as a closed region in the plane $(\rho,P_\rho)$ bounded by the curves $P_\rho=\pm(2\epsilon+2/\rho-m^2/\rho^2-\frac{1}{4}\rho^2)^{1/2}$. We remark that this limit does not depend on the parameter $\mathcal{F}$. Moreover, it is worth noting that when $\mathcal{F}=0$, the limit of the surface of section corresponds to an equatorial periodic orbit ($z$ and $P_z$ are permanently equal to zero).

We take a constant energy $\epsilon=-1$ because, for a wide range of values of $\mathcal{F}$, the classical orbits are bounded, i.e., the energy remains below the Stark saddle-point energy [16]. The value $\epsilon=-1$ defines a scaled principal quantum number $\hat{n}=1/\sqrt{-2\epsilon}=0.707\,1067$ and a critical scaled magnetic quantum number $\hat{m}_c=\hat{n}/\sqrt{5}=0.316\,2277$, and in accordance with the classical perturbation studies [1,8,9], two different transitions from pure Zeeman effect to Stark effect are expected depending on the value of the parameter $\hat{m}$. For $\hat{m}>\hat{m}_c$ the transition is produced in a natural way: the Zeeman rotational states are gradually replaced by the Stark vibrational states. However, for $\hat{m}<\hat{m}_c$, the transition passes through a teardrop bifurcation [1].

## III. EVOLUTION OF THE POINCARE SURFACES OF SECTION

To begin with, we take two values of $\hat{m}$, namely, $\hat{m}=0.36>\hat{m}_c$ and $\hat{m}=0.25<\hat{m}_c$. For the case $\hat{m}=0.36$, the evolution of the surfaces of section, the corresponding periodic orbits as well as the quasiperiodic orbits for $\mathcal{F}$ varying from 0 to 0.35, are shown in Fig. 1. The sequence begins with the pure Zeeman effect [$\mathcal{F}=0$, Fig. 1(a)]: the surface of section shows a single elliptic (stable) fixed point on the axis $P_\rho=0$, labeled as $C$, that corresponds to an almost circular periodic orbit, also labeled as $C$. This orbit is exactly circular when $\epsilon\to-\infty$. As we already pointed out, the limit of the surface of section corresponds to an equatorial periodic orbit labeled as EQ. The orbits around $C$ execute quasiperiodic rotational motion. From the point of view of quantum mechanics, we may associate these rotational levels with quantum states which wave functions are mainly located on the plane $z=0$: the so-called Cacciani's levels of class III [12–14]. This configuration for the Zeeman effect has been widely described by several authors [3,17].

When the electric field is turned on [$\mathcal{F}=0.1$, Fig. 1(b)], the symmetry of the Zeeman effect is broken and the fixed point $C$ appears displaced from the axis $P_\rho=0$. Accordingly, the nature of this periodic orbit changes, and its eccentricity increases. Furthermore, we observe a new stable fixed point in the upper part of the surface of section. The presence of this fixed point is due to the fact that when $\mathcal{F}\neq 0$, the limit of the surface of section does not correspond to any periodic orbit and, as a consequence, a new fixed point appears in the surface of section. We label this fixed point as EQ. The appearance of this new periodic orbit is not associated with any kind of bifurcation because, when the surface of section is defined on a finite and closed space, orbits can appear and disappear at the boundary [18]. Due to this new configuration, the quasiperiodic orbits around $C$ change in such a way that they belong to a mixed regime of vibrational and rotational states. We associate these levels with quantum states whose wave functions are a mixture of Cacciani's levels of classes III and I. On the other hand, the quasiperiodic orbits around EQ also belong to a different mixed regime of vibrational and rotational states: these levels correspond to quantum states whose wave functions are a mixture of Cacciani's levels of classes III and II. These two classes of motion are kept apart by means of a special kind of separatrix that contains no fixed point: both classes of motion evolve in a smooth way from one class to another [8].

As the parameter $\mathcal{F}$ increases, the described trend continues [see Fig. 1(c)]. Finally, when the Stark effect dominates [see Fig. 1(d) for $\mathcal{F}=0.35$], the fixed points $C$ and EQ reach almost stationary position. The quasiperiodic orbits around these points are vibrational levels: the levels around $C$ belong to Cacciani's class II, and those around EQ belong to Cacciani's class I.

Note that, because of the integrability of the pure Stark effect, its corresponding surface of section would simply give concentric circles and each orbit would contribute with a fixed point. However, in our SQZE formulation even an infinitesimal $\gamma$ value (i.e., $\mathcal{F}\to\infty$, $\epsilon\to-\infty$) is enough to change the phase space structure of the pure Stark effect.

In the case $m=0.25$, when $\mathcal{F}=0$, the corresponding surface of section appears in Fig. 2(a). This figure shows two different regions of motion; their separatrix passes through a hyperbolic (unstable) fixed point that corresponds to an almost circular periodic orbit labeled $C$. The stable fixed points correspond to two symmetric elliptic orbits, labeled $E1$ and $E2$. The quasiperiodic orbits around $E1$ correspond to the vibrational Cacciani's levels of class I and those around $E2$ with the vibrational Cacciani's levels of class II. On the other hand, quasiperiodic orbits around $C$ correspond to the rotational Cacciani's levels of class III. Because these three kinds of levels have been already depicted for the case $m=0.36$, for the sake of simplicity, we do not represent any picture of quasiperiodic orbits for the present case $m=0.25$.

The presence of the Stark effect brings again a breaking of the Zeeman symmetry. Indeed, for small values of $\mathcal{F}$ ($\mathcal{F}=0.001$), the two separatrix lobes are not symmetric because the upper one shrinks [Fig. 2(b)]. In this way, the stable fixed points $E1$ and $C$ begin to approach each other, and their corresponding periodic orbits $E1$ and $C$ evolve to a common configuration. Consequently, the vibrational levels around $E1$ gradually disappear, while levels around $E2$ remain vibrational of class I. Moreover, we can also detect a change in the nature of the levels around the separatrix. Therefore, while the levels far away from the separatrix stay rotational (class III), the levels near the separatrix present a mixed regime between rotational and vibrational levels.

Once again, as in case $m=0.36$, the limit of the surface of section does not correspond to any periodic orbit. In this way, the equatorial orbit EQ for $\mathcal{F}=0$, is compelled to evolve to a new periodic orbit located, as a fixed point, inside the surface of section. However, this orbit is not at a glance observable. To detect this point, it is necessary to enlarge the aforementioned zone of the surface of section in Fig. 2(b) in order to observe the presence of a like-arch quasiperiodic orbit. It is inside this quasiperiodic orbit where the fixed point EQ is located. To obtain with accuracy the coordinates of the periodic orbit inside, we have developed a method for searching periodic orbits based on the following correlation function $\mathcal{C}(t)$:

$$\mathcal{C}(t)=e^{-[z_i(t)-z_0]^2}e^{-[\rho_i(t)-\rho_0]^2}e^{-[P_{z_i}(t)-P_{z_0}]^2}e^{-[P_{\rho_i}(t)-P_{\rho_0}]^2},\tag{3}$$

where $(\rho_0,z_0,P_{\rho_0},P_{z_0})$ are the initial conditions of an orbit. When $\mathcal{C}(t)$ is applied to a periodic orbit, this function presents isolated peaks with height close to 1 for values of the time $t$ that are multiple of the period $T$. However, when applied to quasiperiodic orbits, the function $\mathcal{C}(t)$ presents several peaks with height smaller than 1. The application of the function (3) to a set of orbits with initial conditions over a grid of points on the surface of section in Fig. 2(b), allows us to obtain the coordinates of the periodic orbit EQ for $\mathcal{F}=0.001$, which corresponds to an almost equatorial orbit.

When $\mathcal{F}$ increases, the described trend of the points $E1$ and $C$ continues, in such a way that when $\mathcal{F}=0.0025$, the upper separatrix lobe has almost disappeared, causing the collapse between periodic orbits $E1$ and $C$. Accordingly, the vibrational character of the outer levels near the separatrix increases.

Finally, when the Stark parameter reaches the value $\mathcal{F}=0.005$, the collapse between equilibria has occurred, and equilibria $E1$ and $C$ disappear [see Fig. 2(c)]. A *saddle-node* bifurcation takes place. Note that this bifurcation may be associated with the *teardrop* bifurcation accounted by Deprit *et al.* [1] in the normalized problem, which was also intuited, for concrete values of the quantum numbers $m$ and $n$, by Waterland *et al.* [8], Uzer *et al.* [19], and Farrelly *et al.* [9]. As a consequence of this bifurcation, the vibrational levels of class I around $E1$ disappear.

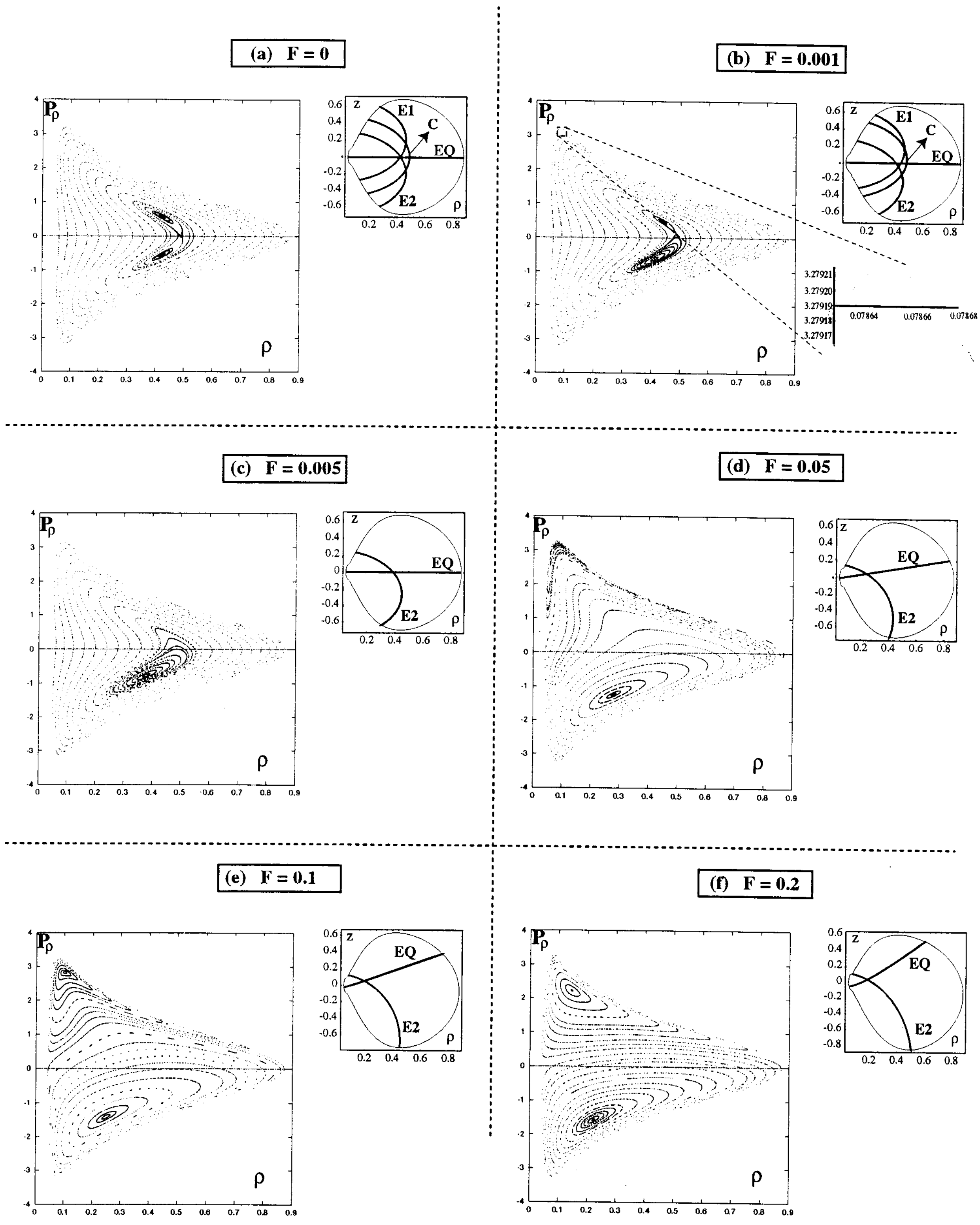


FIG. 2. Evolution of the Poincaré surfaces of section and periodic orbits as a function of the parameter $\mathcal{F}$ for $m=0.36$ and $\epsilon=-1$.

After the *saddle-node* bifurcation, as the influence of the Stark effect increases, the evolution of the surfaces of section is similar to that found in the case $m>m_c$ [see Figs. 2(d)–2(f)]. However, it is necessary that $\mathcal{F}$ reaches values greater than 0.05 in order that the fixed point EQ clearly appears in the surface of section. Finally, when $\mathcal{F}$ takes the value 0.2, the Stark configuration is reached [see Fig. 2(f)].

### IV. NUMERICAL VERSUS ANALYTICAL RESULTS

The evolution of the Poincaré surfaces of section described above matches qualitatively well with the evolution obtained in the work of Deprit *et al.* [1] by means of perturbative methods, for both $m<m_c$ and $m>m_c$. There is a direct correspondence between fixed points in the surfaces of

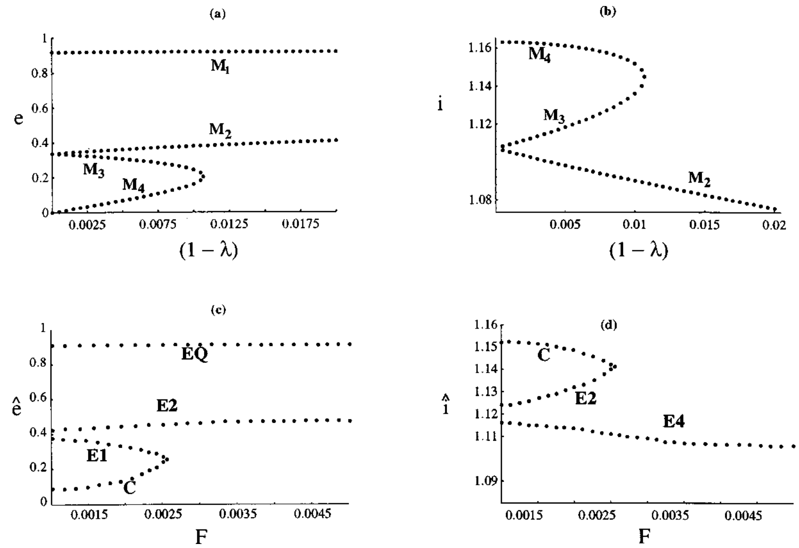


FIG. 3. Comparison of the dimensionless orbital elements of the periodic orbits appearing in the normalized (a), (b) and in the complete (c), (d) problems near the bifurcation.

section and the equilibria in the normalized phase space. Moreover, the saddle-node bifurcation observed for $m<m_c$ accounts for the *teardrop* bifurcation reported in [1].

In order to highlight this correspondence, we pay attention to the evolution of the dimensionless orbital elements of the periodic orbits represented by the fixed points on the surfaces of section and the equilibria of the normalized problem. That is to say, we will show that this correspondence is not only qualitative but quantitative. The dimensionless orbital elements are the eccentricity $e$ and the inclination $i$. We will follow a similar scheme used by Lara *et al.* [20] to corroborate the existence of frozen orbits for the zonal satellite problem [21].

It is worth noting that while each equilibrium of the normalized problem represents a Keplerian orbit, the periodic orbits on the surfaces of section are ''quasi-Keplerian.'' In this way, for each periodic orbit on the surface of section we take the ''mean Keplerian orbit'' by averaging the orbital elements

$$\hat{e}=\int_0^T e(t)dt, \quad \hat{i}=\int_0^T i(t)dt,$$

where $e(t)$ and $i(t)$ are derived from the instantaneous Runge-Lenz vector $\mathbf{A}$ and the angular momentum $\mathbf{L}$ (see, for instance, the work of Delos *et al.* [22]).

For the further discussion, we note that there is not an exact correspondence between the parameters that control the respective influence of electric and the magnetic field in the numerical and in the normalized studies. While $\lambda=0$ in the normalized problem[1] indicates that there is no magnetic field, this situation is not possible for the numerical study, unless $\mathcal{F}\to\infty$. This is the reason why we focus on the values of the orbital elements and not on the values of the parameters $\lambda$ and $\mathcal{F}$.

We perform the comparison of results for the case $m=0.28<m_c$. This value of $m$ yields a value of $\beta=\hat{m}/\hat{n}=0.395\,9798$ in the normalized case. Because in both studies the same bifurcation takes place, we guess the existence of ''critical'' values of eccentricity and inclination associated with this bifurcation. In this way, it is convenient to study the evolution of $e$ and $i$ around the values of $\lambda$ and $\mathcal{F}$ for which the bifurcation occurs. In this sense, we analyze the behavior of the eccentricity and the inclination when $0.98\leqslant\lambda\leqslant1$ and $0\leqslant\mathcal{F}\leqslant0.005$.

In Figs. 3(a) and 3(b) we observe the evolution of the eccentricity and the inclination of the equilibria in the normalized study. We observe that, in both cases, the eccentricity and the inclination of the orbits taking part in the teardrop bifurcation come into coincidence. The critical values of eccentricity and inclination are $e_c=0.203$ and $i_c=1.145$.

Finally, Figs. 3(c) and 3(d) show the evolution of the eccentricity and inclination of the equilibria in the numerical study. In this figure, we observe qualitatively the same evolution as in Figs. 3(a) and 3(b). A more detailed observation reveals that the critical values for which the saddle-node bifurcation takes place are $\hat{e}_c=0.222$ and $\hat{i}_c=1.141$, which are in a good agreement with those already found for the normalized study. Similar good agreement is obtained for values of the eccentricity and inclination of the rest of the periodic orbits.

## V. CONCLUSIONS

We have shown that the transition from the pure Zeeman effect to the Stark effect is produced by a saddle-node bifurcation. Moreover, a remarkable analogy between the phase-

[1]In the normalized problem $0\leqslant\lambda\leqslant1$ is an adjustable parameter that controls the relative influence of the electric and the magnetic fields: for $\lambda=0$ there is only electric field and for $\lambda=1$ there is only magnetic field.

space structure uncovered by means of surfaces of section and the phase portrait of the normalized Hamiltonian is demonstrated. Finally, we find that the classical electronic structure matches the quantum Stark structure of the hydrogenic diamagnetic structure detected in experimental studies.

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