

On the Regularity and Chaos of the Hydrogen Atom Subjected to External Fields

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Abstract

In this paper, the integrable classical case of the Hydrogen atom subjected to three static external fields is investigated. The structuring and evolution of the real phase space are explored. The bifurcation diagram is found and the bifurcations of solutions are discussed. The periodic solutions and their associated periods for singular common-level sets of the first integrals of motion are explicitly described. Numerical investigations are performed for the integrable case by means of Poincaré surfaces of section and comparing them with nearby living nonintegrable solutions, all generic bifurcations that change the structure of the phase space are illustrated; the problem can exhibit regularity-chaos transition over a range of control parameters of system.

Keywords

Hydrogen Atom, Zeeman Effect, Stark Effect, Van Der Waals Interaction, Hamiltonian System, Integrability, Bifurcation, Chaos, Poincaré Surfaces of Section

1. Introduction

Most natural phenomena are generally governed by nonlinear differential equations, for these problems, we must use different mathematical approaches and computational methods to simplify these systems and to study their integrable like lie algebra, the Painlevé criterion, the Ziglin criterion, the Liouville theorem and the Poincaré sections, because physically integrable systems are rare.

The study of the Hydrogen atom has been recently the focus of many works [1]-[10]. Its great importance lies in its fields of implications in different

branches of physics: solid state physics [11], spectroscopy [12], plasmas physics [13], molecular physics [14], astrophysics [15].

The Hydrogen atom is a simple but very complicated system when introducing external fields. The Hydrogen atom in a static magnetic field is a simple system that can be studied experimentally and theoretically, its dynamics in such a field has been a source of many interesting results in atomic physics over the past two decades [16] [17]. It proves to be a prototype of quantum systems whose classical behavior can show chaotic dynamics [18] [19]. Concrete systems are often modeled using systems with natural parameters. The regularity of the behavior of the system is observed for certain values of the parameters, but usually the behavior of the dynamical system becomes unpredictable.

The Hydrogen atom under the effect of external fields is a complicated, non-separable problem and generally displays chaotic behavior for some combinations of the appropriate parameters. The chaotic appearance results from the fact that, for certain initial conditions, the behavior of the dynamic system becomes unpredictable [20]. The chaos is identified by a high sensitivity to the initial conditions and by the variation of the control parameters of the system. Indeed, a system with n degrees of freedom is regular if there are n independent constants of motion [21]. Most problems involving atoms in external fields are very difficult to study analytically and solutions are difficult to obtain. However, for combinations of appropriate parameters, one can find exact solutions.

The isotropic nonrelativistic Hydrogen atom subjected to three static external fields: a magnetic field, an electric field, and a van der Waals interaction. The Hamiltonien (in units such that $m_e = \hbar = e = a_0 = 1$) can be written as:

$$H = \frac{1}{2}p^{2} - \frac{1}{r} + \alpha \left(x^{2} + y^{2} + \lambda^{2}z^{2}\right) + \gamma \left(x^{2} + y^{2}\right) + \beta z$$
(1)

where $r^2 = x^2 + y^2 + z^2$, $p^2 = p_x^2 + p_y^2 + p_z^2$, and α, λ, γ and β are control parameters representing the magnitude of the applied external fields: α is a constant; γ , measured in units of magnetic field $B_0 = 2.35 \times 10^5 \text{ T}$, controls the quadratic Zeeman effect; β , measured in units of electric field $F_0 = 5.14 \times 10^{11} \text{ V/cm}$, controls the Stark effect; and the a-dimensional number λ controls the anharmonicity associated to the van der Waals interaction [10] [11] [12]. This combined potential is very interesting because of its similarity to the fields seen by an ion confined in a Paul trap [13].

The paper is organized as follows: In Section 2 we briefly review the regularized equations of motion and we bring out that the regular 2D Hamiltonian is equivalent to the motion of two coupled anharmonic oscillators. Section 3 presents a detailed description of the real phase space topology on the bifurcation diagram. For noncritical values of the constants of motion h and f, the regular level sets of the first integrals of motion of a completely integrable Hamiltonian system are composed of tori, according to the Liouville theorem. All generic bifurcations of Liouville tori, corresponding to critical values of the constants of motion h and f will be described, by using Fomenko's surgery. In Section 4 we give explicit periodic solutions and their associated periods for singular common-level sets of the constants of motion. In section 5 we also investigate numerically via Poincaré surfaces of section, the structure and evolution of the phase space for the integrable case, comparing them with nearby living nonintegrable solutions, the problem can exhibit regularity-chaos transition over a range of system control parameters. Finally, Section 6 contains our conclusions.

2. Equations of Motion

The regularized Hamiltonian is obtained by transforming Equation (1) to semiparabolic coordinates and the corresponding momenta, namely,

$$p_{x} = \frac{v\cos(\varphi)}{u^{2} + v^{2}} \frac{v\cos(\varphi)}{u^{2} + v^{2}} p_{u} + \frac{u\cos(\varphi)}{u^{2} + v^{2}} p_{v} - \frac{\sin(\varphi)}{uv} p_{\varphi},$$

$$y = uv\sin(\varphi), \quad p_{y} = \frac{v\sin(\varphi)}{u^{2} + v^{2}} \frac{v\sin(\varphi)}{u^{2} + v^{2}} p_{u} + \frac{u\sin(\varphi)}{u^{2} + v^{2}} p_{v} + \frac{\cos(\varphi)}{uv} p_{\varphi}, \quad (2)$$

$$z = \frac{u^{2} - v^{2}}{2}, \qquad p_{z} = \frac{u}{u^{2} + v^{2}} \frac{u}{u^{2} + v^{2}} p_{u} - \frac{v}{u^{2} + v^{2}} p_{v}.$$

Note that the equations of motion associated with the Hamiltonian (1) have a collision singularity at r = 0, which can be removed with the following change in the independent variable

$$\frac{\mathrm{d}t}{\mathrm{d}\tau} = r = \left(u^2 + v^2\right)$$

After such transformation, the regularized Hamiltonian reads

$$\tilde{H}(u,v) = 2 = \frac{1}{2} \left(p_u^2 + p_v^2 \right) + \frac{p_{\varphi}^2}{2} \left(\frac{1}{u^2} + \frac{1}{v^2} \right) - H \left(u^2 + v^2 \right) + \frac{\alpha \lambda^2}{4} \left(u^6 + v^6 \right) + \frac{\beta}{2} \left(u^4 - v^4 \right) + \left(\alpha + \gamma - \frac{\alpha \lambda^2}{4} \right) \left(u^4 v^2 + u^2 v^4 \right)$$
(3)

In this equation, p_{φ} is a conserved quantity, represents the value of the cyclic integral associated to the cyclic coordinate φ , and we put $p_{\varphi} = l$, with l a constant.

The difference between the Hamiltonian (3) and the Hamiltonian of an ion in a Paul trap is that the total pseudo-energy \tilde{H} is equal to 2, that of a trapped ion is -2 (for details, see Ref. [11]).

The equations of motion associated with $\tilde{H}(u,v)$ in the new time τ are, therefore,

$$\begin{split} \dot{u} &= p_{u}, \\ \dot{p}_{u} &= 2hu - 2\beta u^{3} - 6\frac{\alpha\lambda^{2}}{4}u^{5} + \frac{l^{2}}{u^{3}} - \left(\alpha + \gamma - \frac{\alpha\lambda^{2}}{4}\right) \left(4u^{3}v^{2} + 2uv^{4}\right), \\ \dot{v} &= p_{v}, \\ \dot{p}_{v} &= 2hu + 2\beta v^{3} - 6\frac{\alpha\lambda^{2}}{4}v^{5} + \frac{l^{2}}{v^{3}} - \left(\alpha + \gamma - \frac{\alpha\lambda^{2}}{4}\right) \left(4u^{2}v^{3} + 2u^{4}v\right). \end{split}$$
(4)

the dot denotes derivative with respect to τ .

The Hamiltonian (3) characterizes a two dimensional regularized version of

the real three dimensional system after ignoring the cyclic integral associated to the cyclic coordinate φ , $p_{\varphi} = l = 0$.

The study of the dynamics for Hydrogen atom subjected to external fields is easier to process in two-dimensional standardized version than a three-dimensional; and by removing the Coulomb singularity from the original dynamic system, the regularization procedure facilitates the numerical work. Another practical aspect is that the regular 2D Hamiltonian is equivalent to the motion of two coupled anharmonic oscillators with pseudo-energy is equal to 2, a system for which there are effective tools to make the problem easily exploitable.

3. The Phase Space Topology

The two dimensional regularized Hamiltonian (3) is separable if the relation (5) is verified

$$\alpha + \gamma - \frac{\alpha \lambda^2}{4} = 0 \Leftrightarrow \lambda = \pm 2\sqrt{1 + \frac{\gamma}{\alpha}}$$
(5)

in this case the second integral of motion reads

$$F = f = \frac{\left(u^2 p_v^2 - v^2 p_u^2\right)}{2\left(u^2 + v^2\right)} + \frac{\left(\alpha + \gamma\right)\left(v^6 u^2 - u^6 v^2\right) + 2v^2}{u^2 + v^2} - \beta \frac{\left(v^4 u^2 + u^4 v^2\right)}{2\left(u^2 + v^2\right)} \tag{6}$$

$$F = f = zp_x^2 - xp_xp_z + 1 - \frac{z}{\sqrt{x^2 + z^2}} - 2(\alpha + \gamma)x^2z - \frac{\beta}{2}x^2$$
(7)

It is easy to verify that Equation (2) becomes

$$x = uv, \qquad p_x = \frac{v}{u^2 + v^2} \frac{v}{u^2 + v^2} \sqrt{g_1(u)} + \frac{u}{u^2 + v^2} \sqrt{g_2(v)},$$

$$z = \frac{u^2 - v^2}{2}, \qquad p_z = \frac{u}{u^2 + v^2} \frac{u}{u^2 + v^2} \sqrt{g_1(u)} - \frac{v}{u^2 + v^2} \sqrt{g_2(v)}.$$
(8)

where

$$g_1(u) = p_u^2 = 2\left(2 - f + hu^2 - \frac{\beta}{2}u^4 - (\alpha + \gamma)u^6\right)$$
(9)

$$g_{2}(v) = p_{v}^{2} = 2\left(f + hv^{2} + \frac{\beta}{2}v^{4} - (\alpha + \gamma)v^{6}\right)$$
(10)

in these conditions, the equations of motion are

$$\dot{u} = p_u = \pm \sqrt{g_1(u)},$$

$$\dot{v} = p_v = \pm \sqrt{g_2(v)}.$$
(11)

H = h and F = f are the first integrals of motion, functions of (u, v, p_u, p_v) which are constant along the solutions of Equation (11). The system is called (meromorphically) Liouville integrable or completely integrable.

3.1. The Bifurcation Diagrams and the Admissible Region

In this section we shall give the admissible region on the bifurcation diagrams

and a detailed description of the real phase space topology *i.e.* the topology of the real level sets for all generic constants *h* and *f*.

$$A_{\mathbb{R}} = \left\{ \left(u, v, p_{u}, p_{v} \right) \in \mathcal{R}^{4} : H = h, F = f \right\} \subset \mathcal{R}^{4}$$

For doing that we find first the bifurcation diagram *B* of the problem (12), *i.e.* the set of critical values of the energy-momentum mapping

$$(u,v,p_u,p_v) \rightarrow (H,F)$$

It appears, according to several works carried out in this sense (for details, see Ref. [22]-[27]), that the bifurcation diagram *B* is exactly the discriminant locus of the polynomials $g_1(u)$ and $g_2(v)$ whose coefficients are functions in *h*, *f* and the parameters of the system (α, β, γ) .

$$B = B_1 \cup B_2$$

$$B = \left\{ (h, f, \alpha, \beta, \gamma) \in \mathcal{R}^5 : discr(g_1(u)) = 0 \right\}$$

$$\cup \left\{ (h, f, \alpha, \beta, \gamma) \in \mathcal{R}^5 : discr(g_2(v)) = 0 \right\}$$

It is convenient to consider separately, for some values of the constants α , β and γ , two cases $|\lambda| \ge 2$ and $|\lambda| < 2$, because they generate different structures of the topology of the real level sets $A_{\mathbb{R}}$ and the corresponding Poincaré map.

3.1.1. For the Case $|\lambda| \ge 2$

$$B_{1} = \left\{ (h, f) \in \mathcal{R}^{2} : f = 2, f = \frac{1348}{675} - \frac{h}{15} \pm \frac{2}{675} \sqrt{1 + 45h + 675h^{2} + 3375h^{3}} \right\} \subset \mathcal{R}^{2}$$
$$B_{2} = \left\{ (h, f) \in \mathcal{R}^{2} : f = 0, f = \frac{-2}{675} - \frac{h}{15} \pm \frac{2}{675} \sqrt{1 + 45h + 675h^{2} + 3375h^{3}} \right\} \subset \mathcal{R}^{2}$$
$$(14)$$

The set $\{\mathbb{R}^3 \setminus B\} \cap \{|\lambda| \ge 2\}$ consists of 10 connected components (as it is shown in **Figure 1**). Thus, in each connected component of the set $A_{\mathbb{R}} \setminus B$ the level set $A_{\mathbb{R}}$ has the same topological type, and this latter may be changed only if (h, f) passes through $B \cap \{|\lambda| \ge 2\}$.

Theorem 1. The set $\{\mathbb{R}^3 \setminus B\} \cap \{|\lambda| \ge 2\}$ consists of ten connected components. The sections of these components with the plane $\{\lambda = \text{const.}\}$ are shown on Figure 1. If $(h, f, \lambda) \in \mathbb{R}^3 \setminus B$ the topological type of $A_{\mathbb{R}}$ is (diffeomorphic to) a two-dimensional tori T, to a disjoint union of two-dimensional two-tori 2T, or it is the empty set ϕ as it is shown in Table 1.

Proof. Consider the complexified system

$$A_{\alpha} = \left\{ \left(x, z, p_x, p_z, r \right) \in \alpha^5 : H = h = const., F = f = const., r^2 = x^2 + z^2, r \neq 0 \right\}$$

consider also the hyperelliptic curves $\Gamma_1: \{\omega_1^2 = g_1(u)\}$ and $\Gamma_2: \{\omega_2^2 = g_2(v)\}$ and the corresponding Riemann surfaces R_1 and R_2 of the same genus $j_1 = j_2 = 2$. We obtain the explicit solutions of the initial problem (11) by solving the Jacobi inversion problem [28].

Domain Roots of $g_1(u)$ Roots of	of $g_2(v)$ Accessible region $A_{\mathbb{R}}$
1 0 $v_1 <$	$0 < v_2$ $\emptyset \times [v_1, v_2]$ \emptyset
$2 u_1 < u_2 < 0 < u_3 < u_4 v_1 < 0 < 0 < 0 < 0 < 0 < 0 < 0 < 0 < 0 < $	$0 < v_2 \qquad \qquad \begin{bmatrix} u_1, u_2 \end{bmatrix} \cup \begin{bmatrix} u_3, u_4 \end{bmatrix} \times \begin{bmatrix} v_1, v_2 \end{bmatrix} \qquad 2T$
3 $u_1 < u_2 < 0 < u_3 < u_4$ $v_1 < 0 < 0 < 0 < 0 < 0 < 0 < 0 < 0 < 0 < $	$0 < v_2 \qquad \qquad \begin{bmatrix} u_1, u_2 \end{bmatrix} \cup \begin{bmatrix} u_3, u_4 \end{bmatrix} \times \begin{bmatrix} v_1, v_2 \end{bmatrix} \qquad 2T$
4 $u_1 < 0 < u_2$ $v_1 < 0$	$0 < v_2 \qquad \qquad \begin{bmatrix} u_1, u_2 \end{bmatrix} \times \begin{bmatrix} v_1, v_2 \end{bmatrix} \qquad \qquad T$
5 $u_1 < 0 < u_2$ $v_1 < 0 < 0$	$0 < v_2 \qquad \qquad \begin{bmatrix} u_1, u_2 \end{bmatrix} \times \begin{bmatrix} v_1, v_2 \end{bmatrix} \qquad \qquad T$
6 $u_1 < 0 < u_2$ $v_1 < 0 < 0$	$0 < v_2 \qquad \qquad \begin{bmatrix} u_1, u_2 \end{bmatrix} \times \begin{bmatrix} v_1, v_2 \end{bmatrix} \qquad \qquad T$
7 $u_1 < 0 < u_2$ $v_1 < 0 < 0$	$0 < v_2 \qquad \qquad \begin{bmatrix} u_1, u_2 \end{bmatrix} \times \begin{bmatrix} v_1, v_2 \end{bmatrix} \qquad \qquad T$
8 $u_1 < 0 < u_2$ $v_1 < v_2 < 0 < 0$	$0 < v_3 < v_4$ $[u_1, u_2] \times [v_1, v_2] \cup [v_3, v_4]$ $2T$
9 $u_1 < 0 < u_2$ $v_1 < v_2 < 0$	$0 < v_3 < v_4$ $[u_1, u_2] \times [v_1, v_2] \cup [v_3, v_4]$ $2T$
10 $u_1 < 0 < u_2$	$0 \qquad [u_1,u_2] \times \emptyset \qquad \emptyset$

Table 1. The Topological type of $A_{\mathbb{R}}$, and the admissible set for $(h, f) \in \mathbb{R}^2 \setminus B$.



Figure 1. Bifurcation diagram $B \cap \{\lambda = const.\}$ and the numbering of domains for $|\lambda| \ge 2$.

Thus x, z, p_x, p_z can be expressed in terms of hyperelliptic functions living in the Jacobi variety $\Gamma = \Gamma_1 \otimes \Gamma_2$ (where \otimes is the symmetric product). These functions however are not single valued as can be seen from formulae (8) and (11).

Indeed, to each point on the symmetric product $\Gamma_1 \otimes \Gamma_2$ there correspond two values of (x, z, p_x, p_z) . Thus we define the natural projection

$$\pi: A_{\mathcal{A}} \to \Gamma_1 \otimes \Gamma_2$$

corresponding to the involution *i*

$$i:(x,z,p_x,p_z) \rightarrow (x,z,-p_x,-p_z)$$

the real level sets $A_{\mathbb{R}} = \mathcal{R}e(A_{\alpha})$ is the set of fixed points of the complex conju-

gation on A_{α} :

$$\eta: (x, z, p_x, p_z) \to (\overline{x}, \overline{z}, \overline{p}_x, \overline{p}_z)$$
(15)

Consider also the natural projection ξ on the Riemann surface $R = R_1 \otimes R_2$ given in *u*, *v* coordinates by:

$$\xi: (u,v) \to (\overline{u},\overline{v})$$

It induces an involution on the Jacobi variety and hence on A_{α} by the natural projection π . Formulae (6) and (7) imply that this involution ξ coincides with the complex conjugation (15) on A_{α} the upshot is that in order to describe $A_{\mathbb{R}}$ it is enough to study the projection:

$$\pi : A_{\alpha} \to Jac(R) = \Gamma_1 \otimes \Gamma_2$$

Definition. A connected component of the set of fixed points of η on the curves Γ_1 and Γ_2 is called an oval.

To determine the ovals of Γ_1 and Γ_2 it suffices to study the real roots of the polynomials $g_1(u)$ and $g_2(v)$ for different values of h and f as shown in **Table 1**. Using the formulae (8) and the condition that $(x, z, p_x, p_z) \in \mathbb{R}^4$, we find exactly two admissible ovals whose projections on the u-plane and the v-plane are given by Δ_1 and Δ_2 . The product of the admissible ovals in $\Gamma_1 \otimes \Gamma_2$ and the projection π of $A_{\mathbb{R}}$ such as, $A_{\mathbb{R}} = \pi^{-1} (\Gamma_1 \otimes \Gamma_2) = \Delta_1 \times \Delta_2$, gives:

3.1.2. For the Case $|\lambda| < 2$

$$B_{1}' = \left\{ (h, f) \in \mathbb{R}^{2} : f = 2, f = \frac{484}{243} + \frac{h}{9} \pm \frac{2}{243} \sqrt{1 - 27h + 243h^{2} - 729h^{3}} \right\} \subset \mathbb{R}^{2}$$
$$B_{2}' = \left\{ (h, f) \in \mathbb{R}^{2} : f = 0, f = \frac{-2}{243} + \frac{h}{9} \pm \frac{2}{243} \sqrt{1 - 27h + 243h^{2} - 729h^{3}} \right\} \subset \mathbb{R}^{2}$$

Theorem 2. The set $\{\mathbb{R}^3 \setminus B'\} \cap \{|\lambda| < 2\}$ consists of ten connected components. The sections of these components with the plane $\{\lambda = \text{const.}\}$ are shown on Figure 2. If $(h, f, \lambda) \in \mathbb{R}^3 \setminus B'$ The topological type of $A_{\mathbb{R}}$ is (diffeomorphic to) a two-dimensional tori T, to a disjoint union of cylinders C, or it is the real planes \mathbb{R}^2 as it is shown in Table 2.

3.2. Topology of Singular Level Sets and Bifurcations of Liouville Tori

Suppose now that the constants h, f are changed in such a way that (h, f) passes through the bifurcation diagram B. Then the topological type of $A_{\mathbb{R}}$ may change and the bifurcation of Liouville tori takes place.

For the first case $|\lambda| \ge 2$, According to Fomenko surgery on Liouville tori [29], we can have in our case three types of bifurcation of the level set $A_{\mathbb{R}}$ (see **Table 3**). To prove that, it suffices to look at the bifurcations of roots of the polynomials $g_1(u)$ and $g_2(v)$. The correspondence between bifurcation of roots and Liouville tori is shown in **Figure 3**.



Figure 2. Bifurcation diagram $B' \cap \{\lambda = const.\}$ and the numbering of domains for $|\lambda| < 2$.

00	\rightarrow		\rightarrow	\bigcirc
$[u_1, u_2] \cup [u_3, u_4] [v_1, v_2] 2T$	\rightarrow	$[u_1, 0] \cup [0, u_4]$ $[v_1, v_2]$ $S \times (S \land S)$	\rightarrow	$[u_1, u_4] \\ [v_1, v_2] $
ÔÔ	\rightarrow	00	\rightarrow	Ø
$[u_1, u_2] \cup [u_3, u_4] [v_1, v_2] 2T$	\rightarrow	$ \{u_1 = u_2\} \cup \{u_3 = u_4\} \\ [v_1, v_2] $ 2S	\rightarrow	$ \begin{bmatrix} {}^{\uparrow}\!\!\!\! u_1 & {}^{\uparrow}\!\!\!\! u_3 \\ {}^{\downarrow}\!\!\!\! u_2 & {}^{\downarrow}\!\!\!\! u_4 \\ [v_1, v_2] \\ \emptyset $
\bigcirc	\rightarrow	0	\rightarrow	Ø
$egin{array}{l} [u_1, u_2] \ [v_1, v_2] \end{array} \ egin{array}{l} egin{array}{l} egin{array}{l} v_1, v_2 \end{array} \end{bmatrix} \ egin{array}{l} egin{array}{l} egin{array}{l} egin{array}{l} v_1, v_2 \end{array} \end{bmatrix} \end{array}$	→	$ \{ u_1 = u_2 \} \\ [v_1, v_2] $	\rightarrow	$\begin{bmatrix} {}^{\ddagger} u_1 \\ {}^{\downarrow} u_2 \\ [v_1, v_2] \\ \emptyset \end{bmatrix}$

Figure 3. Correspondence between bifurcation sets for $(h, f) \in B$ and bifurcation of invariant Liouville tori, where $(S \wedge S)$ is a union of two circles having exactly one common point.

Table 2. The topological type of $A_{\mathbb{R}}$, and the admissible set for $(h, f) \in \mathbb{R}^2 \setminus B'$.

Domain	Accessible region	$A_{_{ m I\!R}}$
1'	$]{-\infty,u_1}]{\bigcup}[u_2,{+\infty}[\times]{-\infty,+\infty}[$	$2\mathcal{R}^2$
2'	$]-\infty,u_1] \cup [u_2,+\infty[\times]-\infty,+\infty[$	$2\mathcal{R}^2$
3'	$]-\infty,u_{_{1}}]\cup[u_{_{2}},+\infty[\times]-\infty,v_{_{1}}]\cup[v_{_{2}},v_{_{3}}]\cup[v_{_{4}},+\infty[$	$2C + 4\mathcal{R}^2$
4'	$]-\infty, u_1] \cup [u_2, u_3] \cup [u_4, +\infty[\times] -\infty, v_1] \cup [v_2, v_3] \cup [v_4, +\infty[$	$T + 4C + 4\mathcal{R}^2$

Continued		
5'	$]-\infty,u_1]\cup[u_2,u_3]\cup[u_4,+\infty[\times]-\infty,+\infty[$	$C + 2\mathcal{R}^2$
6'	$\left] - \infty, + \infty \right[\times \left] - \infty, + \infty \right[$	\mathcal{R}^{2}
7'	$]-\infty,+\infty[\times]-\infty,v_1]\cup[v_2,v_3]\cup[v_4,+\infty[$	$C + 2\mathcal{R}^2$
8'	$]-\infty,u_1]\cup[u_2,u_3]\cup[u_4,+\infty[\times]-\infty,v_1]\cup[v_2,+\infty[$	$2C + 4\mathcal{R}^2$
9'	$]-\infty,+\infty[\times]-\infty,\nu_1]\cup[\nu_2,+\infty[$	$2\mathcal{R}^2$
10'	$]-\infty,+\infty[\times]-\infty,v_1]\cup[v_2,+\infty[$	$2\mathcal{R}^2$

Table 3. Generic bifurcations of the level set $A_{\mathbb{R}}$.

$6 \rightarrow 1 \\ 6 \rightarrow 10$	$\begin{array}{c} 2 \rightarrow 1 \\ 9 \rightarrow 10 \end{array}$	$2 \rightarrow 5, 9 \rightarrow 10$ $3 \rightarrow 4, 8 \rightarrow 4$
$T \rightarrow \phi$	$2T \rightarrow \phi$	$2T \rightarrow T$

As shown in **Figure 3**, three types of bifurcations of (surgery on) Liouville tori take place:

- 1) Bifurcation $T \rightarrow S \rightarrow \emptyset$: The two dimensional tori *T* is contracted to the circle S corresponding to the periodic solution, and then vanishes.
- Bifurcation 2T → S×(S∧S) → T: The two dimensional two tori 2T merge into two dimensional tori T by passing through the complex S×(S∧S) where (S∧S) is a union of two circles having exactly one common point.
- Bifurcation 2T→2S→Ø: The two dimensional two tori 2T are contracted to two circles 2S corresponding to two periodic solutions, and then vanishes. For the second case |λ|<2, The Fomenko classification of bifurcation of Liouville tori [29] cannot be applied as its invariant level sets contain a non-compact component (cylinder C or plane R²). Thus, we can have the type

To prove that, it suffices to look at the bifurcation of roots of the polynomials $g_1(u)$ and $g_2(v)$ as shown in Figure 4.

of bifurcation of the level set $A_{\mathbb{R}}$ passing from domain *i* to domain *j* in **Table 4**.

4. Periodic Solutions

4.1. For the Case $|\lambda| \ge 2$

When the bifurcation of Liouville tori takes place, the level set $A_{\mathbb{R}}$ becomes completely degenerate. Then we can have exceptional families of periodic solutions. It is seen from **Table 5**, that if (h, f) is on the smooth curves $C_0(C'_0)$ or $C_1(C'_1)$ (see **Figure 5**), $A_{\mathbb{R}}$ contains a isolated circles *S* and 2*S*, respectively which are periodic solutions. Consider now a fixed periodic solution belonging to the curve C_0 . The parameter *v* takes values in the admissible interval $[v_1, v_2]$ and $u = u_1 = u_2$ is equal to the double root of the polynomial $g_1(u)$ (see **Table 5**).



Then we obtain from Equation (8) the following parameterization of fixed periodic solution:

Figure 4. Correspondence between bifurcation of $A_{\mathbb{R}}$ and bifurcation of roots of the polynomials $g_1(u)$ and $g_2(v)$ for differnt values of the invariants (h, f) on the bifurcation diagram B'.



Figure 5. Topological type of $A_{\mathbb{R}}$ for $(h, f) \in B$ and $|\lambda| \ge 2$.

Table 4. Generic bifurcations of the level set A.
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$4' \rightarrow 3'$ $4' \rightarrow 8'$	$\begin{array}{c} 4' \rightarrow 5' \\ 4' \rightarrow 7' \end{array}$	$3' \rightarrow 2' \\ 8' \rightarrow 9'$	$5' \to 6'$ $7' \to 6'$
$T + 4C + 4\mathcal{R}^2 \rightarrow 2C + 4\mathcal{R}^2$	$T + 4C + 4\mathcal{R}^2 \rightarrow C + 2\mathcal{R}^2$	$2C + 4\mathcal{R}^2 \to 2\mathcal{R}^2$	$C+2\mathcal{R}^2\to 2\mathcal{R}^2$

Table 5. Topological type of $A_{\mathbb{R}}$ for $(h, f) \in B$.

Curves	Accessible region	$A_{_{ m R}}$
$C_{_0}$	$\{u_1 = u_2\} \times [v_1, v_2]$	S
C_1	$\{u_1=u_2\}\cup\{u_3=u_4\}\times[v_1,v_2]$	2 <i>S</i>
C_0'	$[u_1, u_2] \times \{v_1 = v_2\}$	S
C'_1	$[u_1, u_2] \times \{v_1 = v_2\} \cup \{v_3 = v_4\}$	2 <i>S</i>

$$\begin{cases} x = 0 \\ z = \frac{-v^2}{2} \end{cases} \begin{cases} p_x = 0 \\ p_z = \pm \frac{\sqrt{g_2(v)}}{v} \end{cases}$$
(16)

to derive the differential equation satisfied by v, we use

$$\frac{\mathrm{d}v}{\mathrm{d}\tau} = p_v$$

we obtain from (10)

$$\frac{\mathrm{d}v}{\sqrt{g_2(v)}} = \pm \mathrm{d}\tau$$

thus $v(\tau)$ and hence $z(\tau)$ can be expressed in terms of hyperelliptic functions.

On the curve C_0 , the second integral of motion f is equal to 2, as well as the characteristic polynomial $g_2(v) = p_v^2 = 2(2 + hv^2 + v^4 - 5v^6)$ depends only on h. Taking this variable change:

$$R = v^{2} \Rightarrow \frac{dR}{2\sqrt{R}} = dv$$
$$d\tau = \pm \frac{dR}{2\sqrt{2}\sqrt{R(2 + hR - 5R^{3} + R^{2})}} = \pm \frac{dR}{2\sqrt{2}\sqrt{P_{2}(R)}}$$
(17)

the polynomial $P_2(R)$ has four distinct roots

$$R_0 = 0$$
, $R_1 = \frac{D^{\frac{1}{3}}}{30} + \frac{2\left(h + \frac{1}{15}\right)}{D^{\frac{1}{3}}} + \frac{1}{15}$, $R_2 = a_0 + ib_0$ et $R_3 = a_0 - ib_0$

where

$$a_{0} = \frac{-D^{\frac{1}{3}}}{60} - \frac{\left(h + \frac{1}{15}\right)}{D^{\frac{1}{3}}} + \frac{1}{15}, \quad b_{0} = \frac{\sqrt{3}}{2} \left[\frac{-D^{\frac{1}{3}}}{60} - \frac{\left(h + \frac{1}{15}\right)}{D^{\frac{1}{3}}}\right]$$
$$D = 180h + 5408 + 60\sqrt{-60h^{3} - 3h^{2} + 540h + 8124}$$

By an inversion of the elliptic integral Equation (17), one explicitly obtains the expression the periodic solution $v(\tau)$:

$$\oint_{0}^{\tau} d\tau = \frac{1}{2\sqrt{2}} \int_{R_{0}}^{R} \frac{dR}{\sqrt{(R-R_{0})(R-R_{1})(R-R_{2})(R-R_{3})}}$$
(18)
$$\tau = n_{0}Cn^{-1}(\cos\varphi, k_{0})$$

where

$$n_0 = \frac{1}{2\sqrt{2A_0B_0}}, k_0 = \frac{R_1^2 - (A_0 - B_0)^2}{4A_0B_0}, \quad A_0^2 = R_1^2 + a_0^2, B_0^2 = b_0^2 + a_0^2$$

 $Cn^{-1}(\cos \varphi, k_0) = F(\varphi, k_0)$ being the incomplete elliptic integral of first kind. The expression of periodic solution $v(\tau)$ is given by solving the Jacobi inversion problem:

$$\tau = \int^{\tau} dt = \int \frac{dv}{\sqrt{g_2(v)}} \Rightarrow v(\tau) = \pm \sqrt{\frac{R_1 B_0 \left\{ Cn \left(2t \sqrt{2A_0 B_0} \right) - 1 \right\}}{\left(A_0 + B_0\right) + \left(A_0 - B_0\right) Cn \left(2t \sqrt{2A_0 B_0} \right)}}$$

The period T_{ν} associated with the solution $\nu(t)$ is obtained by calculating the elliptic integral Equation (17) over the totality of the admissible oval for ν :

$$T_{v} = \oint d\tau = \frac{1}{2\sqrt{2}} \oint \frac{dR}{\sqrt{P_{2}(R)}} = \frac{2}{2\sqrt{2}} \int_{R_{0}}^{R_{1}} \frac{dp_{y}}{\sqrt{R(2 + hR - 5R^{3} + R^{2})}}$$

It's sufficient to replace in Equation (18) the upper bound in the integral by R_1 and multiply by 2, in these conditions $\cos \varphi = -1$, we obtain a period de-

pendent only on the energy *h*:

$$T_{v}(h) = 2n_{0}Cn^{-1}(-1,k_{0}) = 2n_{0}F(\pi,k_{0})$$

where $Cn^{-1}(-1,k_0) = F(\pi,k_0)$ is the complete elliptic integral of the first kind.

In the same way, for the periodic solution on the curve C_1 the parameter v takes values in the admissible oval $[v_1, v_2]$, the double roots of the polynomial $g_1(u)$ are equal to $u_1 = u_2 = -m$ and $u_3 = u_4 = m$ (see Table 5).

The values of the first integrals H and F on the curve C_1 are related by

$$f = \frac{1348}{675} - \frac{h}{15} + \frac{2}{675}\sqrt{1 + 45h + 675h^2 + 3375h^3}$$

From Equation (8) we obtain the following parameterization of fixed periodic solution

$$\begin{cases} x = \pm mv \\ z = \frac{m^2 - v^2}{2} \end{cases} \text{ and } \begin{cases} p_x = \pm \frac{m}{m^2 + v^2} \sqrt{g_2(v)} \\ p_z = \pm \frac{v}{m^2 + v^2} \sqrt{g_2(v)} \end{cases}$$

$$v(t) = \pm \sqrt{\frac{R_1 B_1 \left\{ Cn \left(2t \sqrt{2A_1 B_1} \right) - 1 \right\}}{(A_1 + B_1) + (A_1 - B_1) Cn \left(2t \sqrt{2A_1 B_1} \right)}}$$
(19)

The period of v(t) is

$$T_{v}(h) = 2n_{1}Cn^{-1}(-1,k_{1}) = 2n_{1}F(\pi,k_{1})$$

where

$$n_{1} = \frac{1}{2\sqrt{2A_{1}B_{1}}}, k_{1} = \frac{R_{1}^{2} - (A_{1} - B_{1})^{2}}{4A_{1}B_{1}}, A_{1}^{2} = R_{1}^{2} + a_{1}^{2}, B_{1}^{2} = b_{1}^{2} + a_{1}^{2},$$

$$R_{0} = 0, R_{1} = \frac{1}{15} \left(C^{\frac{1}{3}} + \frac{15h + 1}{C^{\frac{1}{3}}} + 1 \right), a_{1} = \frac{-1}{30} \left(C^{\frac{1}{3}} + \frac{15h + 1}{C^{\frac{1}{3}}} - 2 \right),$$

$$b_{1} = \frac{\sqrt{3}}{30} \left(C^{\frac{1}{3}} - \frac{15h + 1}{C^{\frac{1}{3}}} \right),$$

$$C = 675 \left(1 + \sqrt{(15h + 1)^{3}} \right)$$

$$+ \sqrt{911249 + 20503080h + 307546200h^{2} + 1537731000h^{3} + 911250\sqrt{(15h + 1)^{3}}} \right)$$

From Equation (19), the Cartesian equation for this periodic solution in the (x, z) plan is

$$z(x) = \frac{m^2}{2} - \frac{x^2}{2m^2}$$

4.2. For the Case $|\lambda| < 2$

In this case, it is seen from **Table 6**, that on the smooth curves $L_0(L'_0)$ the

values of the second integral of motion f is equal to 2 (f is equal to 2) (see Figure 6), $A_{\mathbb{R}}$ contains a circles S which correspond to a periodic solutions. On the curve $L_0(f=2)$ the periodic solution v(t) is given by

$$v(t) = \pm \sqrt{\frac{R_1 B_0' \left\{ Cn \left(2t \sqrt{2A_0' B_0'} \right) - 1 \right\}}{\left(A_0' + B_0'\right) + \left(A_0' - B_0'\right) Cn \left(2t \sqrt{2A_0' B_0'} \right)}}$$

The associated period is

$$T_{v}(h) = 2n_{0}'Cn^{-1}(-1,k_{0}') = 2n_{0}'F(\pi,k_{0}')$$

where

$$n_{0}^{\prime} = \frac{1}{2\sqrt{2A_{0}^{\prime}B_{0}^{\prime}}}, k_{0}^{\prime} = \frac{R_{1}^{2} - (A_{0}^{\prime} - B_{0}^{\prime})^{2}}{4A_{0}^{\prime}B_{0}^{\prime}}, A_{0}^{\prime 2} = R_{1}^{2} + a_{0}^{\prime 2}, B_{0}^{\prime 2} = b_{0}^{\prime 2} + a_{0}^{\prime 2}, R_{0} = 0,$$

$$R_{1} = \frac{D_{0}^{\frac{1}{3}}}{18} - \frac{2\left(h - \frac{1}{9}\right)}{D_{0}^{\frac{1}{3}}} - \frac{1}{9}, a_{0} = \frac{-D_{0}^{\frac{1}{3}}}{36} + \frac{\left(h - \frac{1}{9}\right)}{D_{0}^{\frac{1}{3}}} - \frac{1}{9}, b_{0} = \frac{\sqrt{3}}{2}\left(\frac{D_{0}^{\frac{1}{3}}}{18} + \frac{2\left(h - \frac{1}{9}\right)}{D_{0}^{\frac{1}{3}}}\right),$$

$$D_{0} = 108h - 1952 + 36\sqrt{36h^{3} - 3h^{2} - 324h + 2940}$$

Table 6. Topological type of $A_{\mathbb{R}}$ for $(h, f) \in B'$.

Curves	Accessible region	$A_{ m R}$
L_{0}	$]-\infty, u_1] \cup \{u_2 = u_3\} \cup [u_4, +\infty[\times] -\infty, v_1] \cup [v_2, v_3] \cup [v_4, +\infty[$	$S + 2\mathcal{R}_{v} + 2C + 4\mathcal{R}^{2}$
L_0'	$]-\infty, u_1] \cup [u_2, u_3] \cup [u_4, +\infty[\\ \times]-\infty, v_1] \cup \{v_2 = v_3\} \cup [v_4, +\infty[$	$S+2\mathcal{R}_u+2C+4\mathcal{R}^2$



Figure 6. Topological type of $A_{\mathbb{R}}$ for $(h, f) \in B'$ and $|\lambda| < 2$.

5. Numerical Investigation

By making use a set of software routines, implemented in Maple, for plotting 2D projections of Poincaré surfaces of section, method introduced by Poincaré and extended by Hénon [30], we give numerical illustrations of the real phase space topology studied in Section 3. For fixed values of constants h, f, α, λ and β, γ vary, the Liouville tori contained in the level set $\{H = h, F = f\}$ change their topological type, while preserving the integrable behavior of the problem. However, with increasing control parameter associated with magnetic field, the random scattering of points in the sections shows that the system has carried out a transition from regularity through a quasi-regularity to chaotical dynamics.

The Poincaré surfaces of section are plotted in the plane $(q_1, p_1) = (u, p_u)$.

5.1. Regularity-Chaos Transition

Figures 7(a)-(h) represent Poincaré surfaces of section for $\beta = 2$ (electric field) and values of γ (magnetic field) near the integrable case $\gamma = 4$ (from left to right), where for different values of *h* and *f* on the bifurcation diagram *B* the system is totally regular, the topological type of $A_{\mathbb{R}}$ is diffeomorphic to a two-dimensional tori *T*, or a disjoint union of two-dimensional two-tori 2*T*. When the magnetic field increases for $\gamma = 4$ to $\gamma = 4.5$, the corresponding Poincaré surfaces of section show that the system go through a transition from regularity to chaotical dynamics. At $\gamma = 5$ (high magnetic field), all Poincaré surfaces of section show a strong irregular motion, the dynamic is totally chaotic.

Figures 8(a)-(h) show the Poincaré surfaces of section for $\beta = 0$ (no electric field) and $\gamma = 4$, the system still has a regular motion, so we can say that the electric field is not responsible for the chaotic behavior of the system, on the other hand only the variation of the intensity of the magnetic field changes the behavior of the system from regularity to chaotically dynamics.

5.2. Bifurcations of Liouville Tori

Figure 9(a) represents the Poincaré surfaces of section for the bifurcation $2T \rightarrow 2S \rightarrow \phi$, when the system evolves from domain 2 to domain 1 on the bifurcation diagram where the values of the integrals of motion are h = 4.685 and f = 2.221 (blue), 2.524 (black), 2.793 (red), 3.363 (orange), 3.467 (black dot). Figure 9(b) represents the bifurcation $2T \rightarrow 2S \rightarrow \phi$ from domain 9 to domain 10 on the bifurcation diagram where h = 5.437 and f = -1.276 (black), -1.847 (blue), -2.4 (red), -2.587 (black dot). The last values which correspond to black dots are located for $(h, f) \in B$, exactly on the curve of the bifurcation diagram, these black dots present periodic solutions in the form of two isolated circles, because the intersection of a circle with the cutting surface gives a dots. Figures 9(c) represents the bifurcation $2T \rightarrow S \times (S \land S) \rightarrow T$, from domain 3 to domain 4 where h = 8.873 and f = 1.7 (black), 2 (blue), 3.096 (red). Figures 9(d) represent the bifurcation $2T \rightarrow S \times (S \land S) \rightarrow T$, from



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Figure 7. Poincaré surfaces of section for $(h, f) \in \mathbb{R}^2 \setminus B$ and $|\lambda| \ge 2$. The three surfaces (from left to right) correspond to $\beta = 2$ (electric field) and $\gamma = 4, 4.5, 5$ (magnetic field). (a) Domain 2 $(h = 7.477, f = 3.936) A_{\mathbb{R}} \approx 2T$; (b) Domain 3 $(h = 8.873, f = 3.096) A_{\mathbb{R}} \approx 2T$; (c) Domain 4 $(h = 7.155, f = 1.112) A_{\mathbb{R}} \approx T$; (d) Domain 5 $(h = 2.269, f = 1.583) A_{\mathbb{R}} \approx T$; (e) Domain 6 $(h = 0.819, f = 1.011) A_{\mathbb{R}} \approx T$; (f) Domain 7 $(h = 3.021, f = 0.305) A_{\mathbb{R}} \approx T$; (g) Domain 8 $(h = 7.477, f = -1.376) A_{\mathbb{R}} \approx 2T$; (h) Domain 9 $(h = 7.477, f = -2.553) A_{\mathbb{R}} \approx 2T$.



Figure 8. Poincaré surfaces of section for $(h, f) \in \mathbb{R}^2 \setminus B$ and $|\lambda| \ge 2$. The surfaces correspond to $\beta = 0$ (no electric field) and $\gamma = 4$ (magnetic field). (a) Domain 2; (b) Domain 3; (c) Domain 4; (d) Domain 5; (e) Domain 6; (f) Domain 7; (g) Domain 8; (h) Domain 9.



Figure 9. Poincaré surfaces of section on the bifurcation diagram for $(h, f) \in B$ and $|\lambda| \ge 2$.

domain 8 to domain 4 where h = 7.155 and f = -0.738 (black), 0 (blue), 1.112 (orange). Figures 9(e) represents the bifurcation $2T \rightarrow S \times (S \land S) \rightarrow T$, from domain 9 to domain 7 where h = 3.021 and f = -0.569 (black), 0 (red), 0.305 (blue). Figures 9(f) represents the bifurcation $2T \rightarrow S \times (S \land S) \rightarrow T$, from domain 2 to domain 5 where h = 3.88 and f = 1.616 (black), 2 (red), 2.625 (blue). Figures 9(g) represents the bifurcation $T \rightarrow S \rightarrow \phi$, from domain 6 to domain 1 where h = -4.067 and f = 1 (black), 1.437 (blue), 1.891 (red), 2 (black dot). Figures 9(h) represents the bifurcation $T \rightarrow S \rightarrow \phi$, from domain 6 to domain 10 where the values of integrals of motion are h = -4.067and f = 1 (black), 0.5 (blue), 0.2 (red), 0 (black dot). The black dots correspond to the periodic solutions in the form of a isolated circles.

For the case $|\lambda| < 2$, the invariant level sets contain a non-compact component (cylinder *C* or plane \mathcal{R}^2), only in the domain 4' on the bifurcation diagram *B'* we find a single tori.

Figure 10(a) shows the Poincaré sections for $\lambda = \pm \sqrt{3}$ and for a values of the integrals of motion h = -7.879 and f = 0.825 (black), 1.122 (red), 1.758 (blue) corresponding to a point of domain 4' on the bifurcation diagram *B*', where $A_{\mathbb{R}}$ is a two-dimensional tori *T*.

Figure 10(b) shows the Poincaré sections for $\lambda = \pm \sqrt{3}$ corresponding to the bifurcation $T + 4C + 4\mathcal{R}^2 \rightarrow S + 2\mathcal{R}_u + 2C + 4\mathcal{R}^2 \rightarrow 2C + 4\mathcal{R}^2$ from domain 4' to domain 3' on the bifurcation diagram *B*', where the values of the integrals of motion are h = -7.879 and f = 1.9 (black), 2 (black dot), this black dot concerns the periodic solution in the form of a circle.

6. Conclusion

In this paper, we have studied the classical dynamics of the Hydrogen atom in the generalized van der Waals potential subjected to external parallel magnetic and electric fields. By making use of some reductions, the regularized Hamiltonian of the system is described by a two-degree of freedom dependent on certain control parameters. The converted system is equivalent to the motion of two coupled anharmonic oscillators with pseudo-energy easily exploitable. The



Figure 10. Poincaré surfaces of section for different values of, *h*, *f* on the bifurcation diagram B' and $|\lambda| < 2$.

different results obtained show the capacity of the method used to provide precise information on this Hamiltonian system. The very important question that we have studied is the topological analysis of the real invariant manifolds $A_{\mathbb{R}} = \{H = h, F = f\}$ of the system. Fomenko's theory on surgery and bifurcations of the Liouville tori has been combined with that of the algebraic structure to give a rigorous and detailed description of the topology of invariant manifolds $A_{\mathbb{R}}$. For non-critical values of H and F, and for some values of system parameters, we have distinguished two different cases $|\lambda| \ge 2$ where $A_{\mathbb{R}}$ contains torus or is empty. On the other hand, for the case $|\lambda| < 2$, it consists of a torus, or a cylinder or a real plane. Indeed, for the first case, all the components of $A_{\mathbb{R}}$ are compact, while for the second case, they are not compact. Similarly, we have found that Fomenko's theory of the bifurcations of the Liouville tori is applicable to the first case, whereas for the second case, the bifurcations of the tori that appear cannot be described by this theory. It needs to be due to the fact that the Fomenko classification theorem on the bifurcations of the Liouville tori is only valid in the case where the invariant manifold $A_{\mathbb{R}}$ is formed only of compact components. We have also shown how the periodic orbits can be found, how the period of the solutions is determined, and in what ways explicit formulas can be established. Finally, we have also numerically illustrated the generic bifurcations of the Liouville tori and the regularity-chaos transition when one of the control parameters varies. The numerical results show that only the magnetic interaction has affected the dynamic behavior of the Hydrogen atom in parallel magnetic and electric fields. When the magnetic field is weak, the system is totally regular. When the magnetic field is increasing, we observe a transition from regularity to chaotical dynamics. For high magnetic field, the dynamic is totally chaotic.

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