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ON THE CLASSICAL NON-INTEGRABILITY OF THE HAMILTONIAN SYSTEM FOR HYDROGEN ATOMS IN CROSSED ELECTRIC AND MAGNETIC FIELDS

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Abstract. Hydrogen atoms placed in external fields serve as a paradigm of a strongly coupled multidimensional Hamiltonian system. This system has been already very extensively studied, using experimental measurements and a wealth of theoretical methods. In this work, we apply the Morales-Ramis theory of non-integrability of Hamiltonian systems to the case of the hydrogen atom in perpendicular (crossed) static electric and magnetic uniform fields.

1. Introduction. The hydrogen atom placed in external static fields is an example of atomic and fundamentally quantum system, whose classical dynamics may exhibit classically chaotic behaviour [2]. Such dynamical one-electron systems may be studied experimentally [6, 14, 15] as well as by means of quantum chaos theory [2, 3, 16]. Investigation of hydrogen or alkali atoms in a highly excited (the so-called Rydberg) state, interacting with static and uniform magnetic fields gain over recent decades many interest (see e.g. [3]). Such a system however can be considered effectively as a two-dimensional one due to cylindrical symmetry and conservation of the z-component of the angular momentum for an appropriate choice of the gauge for the vector potential of the magnetic field. However, by adding an external and misaligned uniform electric field, one may break down such a cylindrical symmetry. The resulting atomic system interacting with misaligned electric and magnetic fields serves therefore as a truly 3-dimensional system with rich phase-space structure [4]. An enormous amount of theoretical methods (e.g. theoretical classical and quantum, experimental, numerical, perturbative and stability analysis, etc.) have been employed to study that problem (see e.g. [17]).

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Recently, classical dynamics of some systems have been studied in rigorous mathematical terms as far as their integrability is concerned [10, 16] due to a new theorem of Morales-Ramis [12, 13]. For example the non-integrability in the Liouville sense of the classical Zeeman Hamiltonian has been shown by Kummer and Saenz [8], who used an adaptation to the Ziglin analysis [19]. Maciejewski and Przybylska have studied a class of all meromorphically integrable 2D Hamiltonian systems [10]. Also, Mondéjar and Ferrer [11] have discussed the non-integrability of the generalized van der Waals Hamiltonian system recovering the result of [8]. Sawicki and Kuś [16] have studied classical non-integrability of a quantum chaotic Hamiltonian system originating from atomic physics and quantum optics. This study demonstrates the importance of a better understanding of the classical dynamics and its correspondence with the quantum picture for a wide range of systems. This in turn helps to address some fundamental questions within the statistical theory of spectra of quantum systems, whose classical dynamics is chaotic.

The present work is motivated by recent investigations of multidimensional phase space topology in terms of periodic orbits for the hydrogen atom in crossed electric and magnetic fields [4]. The aim is to discuss an application of the Morales-Ramis theorem to the problem of the hydrogen atom in crossed fields. As far as it could be traced back in the literature, integrability of such atomic systems has not been studied yet within the scope of the Morales-Ramis theory. The idea of applying Morales-Ramis theory to study integrability and non-integrability of the system has been also inspired by yet another recent work, where a classical non-integrability for a model Hamiltonian, which takes its origins in atomic physics, has been proved [16]. Approach adopted for the case of crossed electric and magnetic fields will be similar to the method considered for the case of van der Waals Hamiltonian systems [11].

2. Integrability and non-integrability of Hamiltonian systems

2.1. General remarks. Let H be a complex analytical Hamiltonian function of the classical system with n degrees of freedom:

$$H(\mathbf{q},\mathbf{p}), \qquad \mathbf{q}=(q_1,\dots,q_n), \qquad \mathbf{p}=(p_1,\dots,p_n).$$

The canonical equations are given by:

$$\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i}, \\ \dot{p}_i &= -\frac{\partial H}{\partial q_i}, \qquad i=1,\dots,n. \end{aligned}$$

Such a Hamiltonian system is by definition completely integrable or Liouville integrable if there are n integrals of motion, functions $f_1 = H$, $f_2,\dots,f_n$ that are

- functionally independent,
- mutually in involution with respect to the Poisson bracket, $\{f_i, f_j\} = 0$, $i,j = 1,\dots,n$.

2.2. The Morales-Ramis theorem and non-integrability criterion. Consider an n degrees of freedom Hamiltonian system [13, 1]

$$H(\mathbf{p},\mathbf{q}) = T + V = \frac{1}{2}\left(p_1^2 + \ldots + p_n^2\right) + V(q_1,\ldots,q_n),$$

where V is a complex homogeneous function of integer degree $k \neq 0$ and $n \geq 2$.

First, one selects a particular solution $\mathbf{c} = (c_1,\ldots,c_n)$ of the equation with the gradient of the potential

$$\mathbf{c} = V'(\mathbf{c}).$$

The solution $\mathbf{c}$, called a homothetical point (see e.g. [1]), provides a particular solution of the Hamiltonian system (homothetical solution):

$$\dot{\mathbf{q}} = z(t)\mathbf{c},$$

$$\dot{\mathbf{p}} = \dot{z}(t)\mathbf{c},$$

where the scalar function $z(t)$ is a solution of the hyperelliptic differential equation

$$\dot{z}^2 = \frac{2}{k}\left(1 - z^k\right).$$

The homothetical solution allows to compute the variational equation (VE) in its vicinity parametrized with a new variable η:

$$\ddot{\eta} = -z(t)^{k-2}V''(\mathbf{c})\eta.$$

Assuming that the Hessian matrix $V''(\mathbf{c})$ of second partial derivatives is diagonalizable, one may consider its eigenvalues λ_i, $i = 1,\ldots,n$. The eigenvalues $\{\lambda_i\}$ are called Yoshida coefficients [12, 13, 1]. One can note that $\lambda_n = k - 1$.

The Theorem of Morales-Ramis says [13, 1] that if the Hamiltonian system with the homogenous potential of order k is meromorphically completely integrable, then each pair (k,λ_i) has to match one of the items shown in table 1 [13, 1].

Table 1. Theorem of Morales-Ramis: all possible pairs (k,λ_i) for homogeneous integrable potential of integer degree k and eigenvalues $\{\lambda_i\}$ of its Hessian matrix (p-arbitrary integer number) [12, 13] (see also [1])

Pairs (k,λ_i)			
1.	$(k,\ p + p(p-1)\frac{k}{2})$	10.	$(-3,\ \frac{25}{24} - \frac{1}{24}(\frac{12}{5} + 6p)^2)$
2.	$(2,\ z),\ z \in \mathbb{C}$	11.	$(3,\ -\frac{1}{24} + \frac{1}{24}(2 + 6p)^2)$
3.	$(-2,\ z),\ z \in \mathbb{C}$	12.	$(3,\ -\frac{1}{24} + \frac{1}{24}(\frac{3}{2} + 6p)^2)$
4.	$(-5,\ \frac{49}{40} - \frac{1}{40}(\frac{10}{3} + 10p)^2)$	13.	$(3,\ -\frac{1}{24} + \frac{1}{24}(\frac{6}{5} + 6p)^2)$
5.	$(-5,\ \frac{49}{40} - \frac{1}{40}(4 + 10p)^2)$	14.	$(3,\ -\frac{1}{24} + \frac{1}{24}(\frac{12}{5} + 6p)^2)$
6.	$(-4,\ \frac{9}{8} - \frac{1}{8}(\frac{4}{3} + 4p)^2)$	15.	$(4,\ -\frac{1}{8} + \frac{1}{8}(\frac{4}{3} + 4p)^2)$
7.	$(-3,\ \frac{25}{24} - \frac{1}{24}(2 + 6p)^2)$	16.	$(5,\ -\frac{9}{40} + \frac{1}{40}(\frac{10}{3} + 10p)^2)$
8.	$(-3,\ \frac{25}{24} - \frac{1}{24}(\frac{3}{2} + 6p)^2)$	17.	$(5,\ -\frac{9}{40} + \frac{1}{40}(4 + 10p)^2)$
9.	$(-3,\ \frac{25}{24} - \frac{1}{24}(\frac{6}{5} + 6p)^2)$	18.	$(k,\ \frac{1}{2}(\frac{k-1}{k} + p(p+1)k))$

3. The physical model for the crossed fields

3.1. The Hamiltonian. The hydrogen atom in perpendicular (crossed) static and uniform electric and magnetic fields can be cast in the following form, using atomic units [2, 5]:

$$H = \frac{1}{2}\mathbf{p}^2 - \frac{1}{r} + \frac{B}{2}L_z + \frac{B^2}{8}\left(x^2+y^2\right) + Fx, \tag{1}$$

where the magnetic field B placed along the z-direction is in units of 2.35×10^5 T and the electric field F oriented along the x-direction is in units of 5.14×10^9 V/cm.

It can be shown that under appropriate scaling, instead of considering three parameters E, B, F one may have only two scaled parameters $E_0 = B^{-2/3}E$, $F_0 = B^{-4/3}F$, where the scaling factor depends on B.

3.2. The Kustaanheimo–Stiefel transformation. The Kustaanheimo–Stiefel (KS) transformation [9] along with the regularization to a new time variable τ reduces the Hamiltonian (1) of the problem to the system of four coupled anharmonic oscillators. Introduction of new variables $\mathbf{u} = (u_1, u_2, u_3, u_4)$ by the nonlinear KS transformation [9, 5] given by

$$\mathbf{r} = \mathbf{T}\mathbf{u},$$

with

$$\mathbf{T} = \begin{pmatrix} u_1 & -u_2 & -u_3 & u_4 \\ u_2 & u_1 & -u_4 & -u_3 \\ u_3 & u_4 & u_1 & u_2 \\ u_4 & -u_3 & u_2 & -u_1 \end{pmatrix},$$

allows in particular $\mathbf{r} = (x, y, z)$ to be written in the following form:

$$\begin{aligned} x &= 2(u_1u_3 + u_2u_4), \\ y &= 2(u_1u_2 - u_3u_4), \\ z &= u_1^2 - u_2^2 - u_3^2 + u_4^2. \end{aligned}$$

Additionally, there is a constraint on the new conjugate momenta $\mathbf{P}$:

$$L_z = u_4P_1 - u_1P_4 = u_3P_2 - u_2P_3.$$

3.3. The Hamiltonian in four dimensions. Making an additional transformation to a new time τ [5]:

$$\frac{dt}{d\tau} = 4\mathbf{u}^2$$

leads to a new Hamiltonian $\mathcal{H}$:

$$\begin{aligned} 4 = \mathcal{H} = {} & \frac{1}{2}\left(\mathbf{P}^2 + \omega^2\mathbf{u}^2\right) \\ & + 2BL_z\mathbf{u}^2 + 2B^2\mathbf{u}^2(u_1^2+u_4^2)(u_2^2+u_3^2) \\ & + 8F\mathbf{u}^2(u_1u_3 + u_2u_4), \end{aligned} \tag{2}$$

where $\omega^2 = -8E$ and $\mathbf{u}^2 = r = u_1^2 + u_2^2 + u_3^2 + u_4^2$. The Hamiltonian $\mathcal{H}$ describes in fact four one-dimensional and coupled anharmonic oscillators.

4. Application of the Morales-Ramis theorem. In order to prove a complete non-integrability, let us consider the case of physical parameters which obey the constraint

$$\left(\frac{1}{2}\omega^2 + 2BL_z\right)\mathbf{u}^2 = 0.$$

This is equivalent to the choice of the (initial) energy E such that:

$$E = \frac{1}{2}BL_z.$$

A similar reasoning (carried out for a different value of the energy of another physical problem) has been used earlier in [11]. This leads to a simplification of the total system and allows to meet assumptions of the Morales-Ramis theorem with respect to the potential form.

4.1. Homothetical points. The potential V is of degree $k = 6$ and has the form

$$V(\mathbf{u}) = 2B^2\mathbf{u}^2(u_1^2 + u_4^2)(u_2^2 + u_3^2) + 8F\mathbf{u}^2(u_1u_3 + u_2u_4).$$

Therefore, the equations for homothetical points read:

$$\begin{aligned}
0 &= -u_1 + 2(4Fu_3 + 2B^2u_1(u_2^2 + u_3^2))\mathbf{u}^2 \\
&\quad + 4u_1(4F(u_1u_3 + u_2u_4) + B^2(u_2^2 + u_3^2)(u_1^2 + u_4^2)), \\
0 &= -u_2 + 2(4Fu_4 + 2B^2u_2(u_1^2 + u_4^2))\mathbf{u}^2 \\
&\quad + 4u_2(4F(u_1u_3 + u_2u_4) + B^2(u_2^2 + u_3^2)(u_1^2 + u_4^2)), \\
0 &= -u_3 + 2(4Fu_1 + 2B^2u_3(u_1^2 + u_4^2))\mathbf{u}^2 \\
&\quad + 4u_3(4F(u_1u_3 + u_2u_4) + B^2(u_2^2 + u_3^2)(u_1^2 + u_4^2)), \\
0 &= -u_4 + 2(4Fu_2 + 2B^2u_4(u_2^2 + u_3^2))\mathbf{u}^2 \\
&\quad + 4u_4(4F(u_1u_3 + u_2u_4) + B^2(u_2^2 + u_3^2)(u_1^2 + u_4^2)).
\end{aligned} \tag{3}$$

In order to find a solution of the above equations, we first consider a lemma.

LEMMA 4.1. *The Hamiltonian system (2) of crossed electric and magnetic fields for a choice of parameters such that $\omega^2/2 + 2BL_z = 0$, has homothetical points which satisfy*

$$u_1u_2 = u_3u_4. \tag{4}$$

Proof. Subtracting the fourth equation of the set (3) multiplied by u_1 from the first equation of the set (3) multiplied by u_4 one gets (the same when the third equation multiplied by u_2 is subtracted from the second multiplied by u_3):

$$8F(-u_1^3u_2 + u_1^2u_3u_4 + (u_3u_4 - u_1u_2)(u_2^2 + u_3^2 + u_4^2)) = 0.$$

By substituting u_3u_4 with u_1u_2 one verifies that the above equation is satisfied. Thus the solutions of (3) have to obey the condition $u_1u_2 = u_3u_4$. ■

REMARK. Note that the condition (4) corresponds to $y = 0$ in Cartesian coordinates.

Let us now take a particular case which obeys the condition (4):

$$u_1 = u_3, \qquad u_2 = u_4. \tag{5}$$

Note that for such a choice, it follows that $\mathbf{u}^2 = 2(u_1^2 + u_2^2)$ and $r = \mathbf{u}^2 = x$. Therefore $z = 0$. This means that the desired homothetical points are situated along the direction of the electric field (x axis in Cartesian coordinates).

In the special case (5) the equation set (3) reduces to

$$\begin{aligned}(-1 + 16F\mathbf{u}^2 + 3B^2\mathbf{u}^4)u_1 &= 0,\\ (-1 + 16F\mathbf{u}^2 + 3B^2\mathbf{u}^4)u_2 &= 0.\end{aligned}$$

It has a nontrivial solution when

$$-1 + 16F\mathbf{u}^2 + 3B^2\mathbf{u}^4 = 0.$$

Choosing $u_1 = u_2$, it follows finally that a homothetical point is

$$c = u_1 = u_2 = u_3 = u_4 = \pm\sqrt{-\frac{2F}{3B^2} + \frac{\sqrt{3B^2 + 64F^2}}{12B^2}}. \tag{6}$$

4.2. Eigenvalues of the Hessian for a homothetical point. By denoting

$$\begin{aligned}\alpha &= 32c^2(2B^2c^2 + F),\\ \beta &= 64c^2(B^2c^2 + F),\\ \gamma &= 16c^2(5B^2c^2 + 4F),\\ \delta &= 32c^2(B^2c^2 + F) = \beta/2,\end{aligned}$$

one may cast the Hessian matrix in the form

$$\mathbf{V}''(\mathbf{c}) = \begin{pmatrix} \gamma & \alpha & \beta & \delta \\ \alpha & \gamma & \delta & \beta \\ \beta & \delta & \gamma & \alpha \\ \delta & \beta & \alpha & \gamma \end{pmatrix}.$$

The eigenvalues (Yoshida coefficients) of the Hessian matrix are

$$\lambda = \{-16B^2c^4, 48B^2c^4, 16c^2(3B^2c^2 + 4F), 48c^2(5B^2c^2 + 4F)\}.$$

Taking the eigenvalues for the Hessian matrix at the homothetical point

$$c^2 = -\frac{2F}{3B^2} + \frac{\sqrt{3B^2 + 64F^2}}{12B^2},$$

one gets the following explicit formulas for the eigenvalues:

$$\left\{ -\frac{(-8F + \sqrt{3B^2 + 64F^2})^2}{9B^2}, \frac{(-8F + \sqrt{3B^2 + 64F^2})^2}{3B^2}, \right.$$
$$\left. 1, \frac{15B^2 + 32F(8F - \sqrt{3B^2 + 64F^2})}{3B^2} \right\}.$$

Since $k = 6$, according to the theorem of Morales-Ramis it remains to check if all of these eigenvalues are described by one of these families:

$$\left(6, p + 3p(p-1)\right), \qquad \left(6, \frac{1}{2}\left(\frac{5}{6} + 6p(p+1)\right)\right). \tag{7}$$

It is easy to see that for a generic case (most of real values of F and B) the eigenvalues found could not be written as an integer or a rational number of the form (7). Thus at fixed energy the Hamiltonian system for crossed electric and magnetic fields is not completely integrable.

Note that even taking $F = 0$ (only magnetic field present, quadratic Zeeman effect) the Hessian eigenvalues read

$$\left\{-\frac{1}{3}, 1, 1, 5\right\}.$$

The pair $(6, -1/3)$ is obviously not of the form given by (7). Therefore the Hamiltonian system with only magnetic field is not completely integrable either. Thus we recover the result of [8, 11].

For the crossed fields problem, some eigenvalues in general are irrational numbers and therefore are not of the form given by (7). Therefore in conclusion, the Hamiltonian system is not completely integrable by independent meromorphic integrals in involution. Since there is not a complete system of meromorphic integrals, in particular there is no complete system of analytic integrals for the crossed fields problem.

5. Conclusions. In this work, the criterion provided by the Morales-Ramis theorem has been applied to the Hamiltonian system describing a classical hydrogen atom in external uniform and static magnetic and electric fields, which are perpendicular to each other. The present study shows a certain property of the homothetical point for a family of parameters (e.g. energies). This property allows to show that the Hamiltonian system considered is generally not integrable in Liouville sense.

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