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Non-integrability proof of the frozen planetary atom configuration

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Abstract

We give a computer-aided proof of the non-integrability of an important collinear configuration of the three-body problem in atomic physics. We consider the configuration of helium-like atoms where two electrons are on the same side of the atom. Numerical evidence shows that this configuration for helium atom has a Poincaré section that is hardly distinguishable from an integrable system. We extend the model for several helium-like atoms with different values of Z and also consider the case where a heavier particle takes the place of an electron, such as the muon.

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1. Introduction

The three-body problem, either Coulombian or gravitational, is one of the most important problems in physics. The two-electron atoms, e.g., the helium atom, form a subclass of that problem. The helium atom is a model to study the classical, semiclassical and quantum mechanics of a generic non-integrable system [1]. Despite that generic non-integrability, there are some restricted configurations of the helium atom which show stability that is similar to an integrable system, e.g., the special regime known as the *frozen planetary atom* (FPA) [2–4].

The FPA configuration has been observed experimentally [5] and numerically [6]. The FPA can be reduced to one dimension (1D) motion (collinear approximation) where it is characterized by the outer electron remaining at an approximately fixed distance from the nucleus while the inner electron oscillates. In the 2D picture, the inner electron is in Keplerian motion around the nucleus; the inner electron also precesses with opposite angular momentum in relation to the Kepler motion. The outer electron follows the inner electron with angular momentum in the same direction as the inner precession motion and with the opposite direction



Figure 1. A typical trajectory of two resonant electrons which justifies the frozen planetary atom.

to the Kepler one [7]. The 2D FPA is shown in figure 1. The configuration of the atom in that motion is near to a streamline and allows for the reduction to a 1D motion known as the FPA.

Numerical evidence shows that the FPA configuration in 1D has a Poincaré section hardly distinguishable from an integrable system [3]. We give a proof of the non-integrability in order to solve this important question.

The 1D Hamiltonian is shown below

$$H = \frac{1}{2} \left(p_1^2 + p_2^2 \right) - \frac{Z}{|x_1|} - \frac{Z}{|x_2|} + \frac{1}{|x_1 - x_2|}$$
(1)

where x_i is the position of the *i*th electron in Cartesian coordinates and p_i is the corresponding momentum. We obtain the two degrees of freedom Hamiltonian (1) in the approximation where the nucleus (*Z*) has infinite mass. The 1D Hamiltonian with two electrons on the same side of the atom is shown below

$$H = \frac{1}{2} \left(p_1^2 + p_2^2 \right) - \frac{Z}{|x_1|} - \frac{Z}{|x_2|} + \frac{1}{||x_1| - |x_2||}.$$
 (2)

The motion derived from equation (2) is stable. The invariant tori of this nearly integrable system are centred on a stable periodic orbit where the outer electron barely moves. We show below the Poincaré section for this approximation in figure 2(*a*) [8]. In figures 2(*b*) and (*c*) an electron has been substituted by a heavier particle. If that particle is near the nucleus (figure 2(*b*)), the section shows evidence of non-integrability before the value of $m_{\mu}/m_e = 200$ is reached, i.e. muon mass. If the situation is inverted (figure 2(*c*)), we have the same island of stability as the helium atom (figure 2(*a*)). Richter *et al* [9] found that the FPAs exist for all two electron atoms or ions with nuclear charges $1 < Z < \infty$. They found that the collinear periodic orbit of this configuration is fully stable for nuclear charges $Z \leq 12.786$, which guarantees the existence of long-lived resonances for the sequence (isoelectronic) $1 < Z \leq 12$. We also examine this sequence of Z values and find that none of them are integrable.

If one of the electrons is substituted by a heavier particle with the same electron charge, the 1D Hamiltonian for a helium-like atom (Z = 2) [8] is

$$H(r_1, r_2, p_1, p_2) = \frac{p_1^2}{2\mu_{12}} + \frac{p_2^2}{2\mu_3} + \left[-\frac{2}{|r_1|} - \frac{2}{|r_2 + \frac{m_2}{m_1 + m_2}r_1|} + \frac{1}{|r_2 - \frac{m_1}{m_1 + m_2}r_1|} \right]$$
(3)



Figure 2. Poincaré section (r_2, p_2) , E = -1, $r_1 = 0$ and $p_1 > 0$ for the one-dimensional atom $(a) \alpha - e - e$; $(b) \alpha - m_2 - e$, $m_2/m_e = 30$; $(c) \alpha - e - \mu$ (see equation (3) for notation).

where the reduced masses are: $\mu_{12} = \frac{m_1 m_2}{m_1 + m_2}$ and $\mu_3 = \frac{m_3 (m_1 + m_2)}{m_1 + m_2 + m_3}$, where $m_3 = m_{\alpha}$ and m_i , i = 1, 2 are either the pair electron-heavier particle or vice versa.

The case for the electron-muon and vice versa was studied in [8] and is shown in figure 2. As mentioned before, the sequence $\mu - e$ is obviously not integrable, but the $e - \mu$ is as regular as the e - e case. So, after varying the Z value according to [9] we prove numerically that $\mu - e$, $\pi - e$, k - e and $\bar{p} - e$ (and vice versa) are not integrable.

2. Morales-Ramis method for homogeneous potentials

Yoshida's theorem [10] for a homogeneous potential and for two degrees of freedom (n = 2) is a nice algorithmical version of the involved algebraic Ziglin theorem using monodromy groups. The following theorem due to Morales-Ramis [11] is a generalization of Yoshida's theorem for more than two degrees of freedom, and without its limitations at resonances.

We offer below a quick description of the theorem which we believe necessary for the understanding of the steps of the proof of non-integrability of the FPA. We apply the Morales-Ramis theorem varying Z and changing one electron for a heavier particle with the same charge, such as a muon.

Consider the Hamiltonian $H(\mathbf{p}, \mathbf{q}) = \mathbf{p}^2/2 + V(\mathbf{q})$, where $\mathbf{q} = (q_1, \dots, q_n)$ and $\mathbf{p} = (p_1, \dots, p_n)$. For other types of Hamiltonians with homogeneous $V(\mathbf{q})$ and more general Hamiltonians, see [11]. If $V(\mathbf{q})$ is a homogeneous potential of degree k, $V(a\mathbf{q}) = a^k V(\mathbf{q})$, there exists a particular solution of the corresponding Hamilton equations as follows:

$$q_i = c_i f(t)$$
 $p_i = c_i \dot{f}(t)$ $i = 1, ..., n.$ (4)

The f are solutions of the differential equation

$$\dot{f}^2 = \frac{2}{k}(1 - f^k)$$
 $k \neq 0$

Then, it is easy to see that c_i are solutions of the *n* equations given by

$$c_j = \frac{\partial V}{\partial q_j}(c_1, \dots, c_n)$$
 $j = 1, \dots, n$

The linear variational equations (VE) of the system around the above particular solution are given by

$$\ddot{\eta} = -f(t)^{k-2} \frac{\partial^2 V}{\partial q_i \partial q_j}(\mathbf{c}) \eta$$

The VE can be expressed as a direct sum of n second-order equations:

$$\ddot{\xi} = -f^{k-2}(\lambda_i)\xi \qquad i = 1, \dots, n$$

where the λ_i are the eigenvalues of the Hessian matrix, which are called Yoshida's integrability coefficients. The equation with i = n, corresponding to the eigenvalue $\lambda_n = k - 1$, is the tangential variational equation which is trivially solvable. We call NVE n - 1 remaining equations. By the symmetries of this problem the NVE is a system of independent hypergeometric differential equations in the independent variable $q = f^k$. Then we write $ANVE_i$ for the scalar second-order differential equation corresponding to Yoshida's integrability coefficients λ_i :

$$ANVE_i = ANVE_1 + ANVE_2 + \dots + ANVE_{n-1}$$

is a second-order differential equation formed by the sum of the remaining equations, and is solvable if and only if each $ANVE_j$ is solvable. This means that the identity component of the Galois group of the ANVE system is solvable if each identity component of the Galois group of the $ANVE_j$, j = 1, 2, ..., n - 1, is solvable.

To summarize, we express this sum by finding the numbers $\lambda = \text{Tr}(\text{Hess } V) - (k - 1)$ and find whether the pair (k, λ) is in accordance with one of the necessary conditions of the following theorem:

Theorem 1. A necessary condition for a Hamiltonian system, with a homogeneous potential of degree k, to be completely integrable with (holomorphic or meromorphic) first integrals, is that each pair (k, λ_i) belongs to one of the following list (with the exception of the trivial case k = 0):

- (1) (k, p + p(p 1)k/2),
- (2) (2, arbitrary complex number),
- (3) (-2, arbitrary complex number),
- (4) $\left(-5, \frac{49}{40} \frac{1}{40}\left(\frac{10}{3} + 10p\right)^2\right),$
- (5) $\left(-5, \frac{49}{40} \frac{1}{40}(4+10p)^2\right)$,
- (6) $\left(-4, \frac{9}{8} \frac{1}{8}\left(\frac{4}{3} + 4p\right)^2\right)$,
- (7) $\left(-3, \frac{25}{24} \frac{1}{24}(2+6p)^2\right)$,
- (8) $\left(-3, \frac{25}{24} \frac{1}{24}\left(\frac{3}{2} + 6p\right)^2\right)$,
- (9) $\left(-3, \frac{25}{24} \frac{1}{24}\left(\frac{6}{5} + 6p\right)^2\right)$,
- (10) $\left(-3, \frac{25}{24} \frac{1}{24}\left(\frac{12}{5} + 6p\right)^2\right)$,
- (11) $(3, -\frac{1}{24} + \frac{1}{24}(2+6p)^2),$
- (12) $(3, -\frac{1}{24} + \frac{1}{24}(\frac{3}{2} + 6p)^2),$
- (13) $\left(3, -\frac{1}{24} + \frac{1}{24}\left(\frac{6}{5} + 6p\right)^2\right)$,
- (14) $\left(3, -\frac{1}{24} + \frac{1}{24}\left(\frac{12}{5} + 6p\right)^2\right)$,
- (15) $\left(4, -\frac{1}{8} + \frac{1}{8}\left(\frac{4}{3} + 4p\right)^2\right)$,
- $(16) \ \left(5, -\frac{9}{40} + \frac{1}{40} \left(\frac{10}{3} + 10p\right)^2\right),$
- $(17) \ \left(5, -\frac{9}{40} + \frac{1}{40}(4+10p)^2\right),$
- $(18) \left(k, \frac{1}{2}\left(\frac{k-1}{k} + p(p+1)k\right)\right)$

where p is an arbitrary integer.

3. Application to several frozen planetary approximations

3.1. Non-interacting two-electron model

In this trivially integrable case we will find that it is possible to obtain a pair (k, λ) which satisfies theorem 1. Then, we add the interaction term which will break this integrability. Our first step in the application of the Morales-Ramis integrability theorem (or rather, non-integrability theorem) is the evaluation of the vectors c_1 and c_2 as the solutions of the system of equations:

$$\frac{\partial V(c_1, c_2)}{\partial c_i} = + \frac{Z}{c_i^2} = c_i \Rightarrow c_i = Z^{1/3}.$$
(5)

The degree of homogeneity is k = -1. So there are only two cases in theorem 1 where k can take any value, namely the first and last one, which are

i)
$$p - p(p-1)/2 = \lambda$$
 (ii) $+1 - p(p+1)/2 = \lambda$. (6)

 $\lambda = \text{Tr}(\text{Hess } V) - (k - 1)$, where Hess is the Hessian matrix of $V(x_1, x_2)$ evaluated at the solutions c_1 and c_2 of equations (5). The Hessian matrix is Hess = -2I, where *I* is the identity matrix from which we can calculate the values of $\lambda = \text{Tr}(\text{Hess}) - (k - 1) = -2$.

We evaluated (i) and (ii) for a set of integers p: from (i) the integers are -1 and 4 and from (ii) the integers are -3 and 2. Therefore, the necessary condition for integrability given by the theorem above is satisfied.

We note that this is not a proof of integrability since the condition stated by theorem 1 is a necessary condition only. The theorem works at its best when this necessary condition is not satisfied, because in this case we can be sure that the system being discussed is then non-integrable. Indeed, this is the case for the particular perturbations that we treat in the next two subsections.

3.2. Helium-like atoms (variable Z)

Now, we add the interaction term which will break the integrability of the above example. As before, our first step is the evaluation of the vectors c_1 and c_2 :

$$\frac{\partial V(c_1, c_2)}{\partial c_1} = \frac{Z}{c_1^2} + \frac{1}{(c_2 - c_1)^2} = c_1 \qquad \frac{\partial V(c_1, c_2)}{\partial c_2} = \frac{Z}{c_2^2} - \frac{1}{(c_2 - c_1)^2} = c_2.$$
(7)

The degree of homogeneity is still k = -1. So the pair (k, λ) used in the necessary condition for integrability are still given by equations (6).

In the problem at hand, the value of λ is the trace of the Hessian matrix of $V(r_1, r_2)$, evaluated at the solutions c_1 and c_2 of equations (7), minus (k - 1) = -2 as before. The Hessian matrix is

$$\begin{bmatrix} -2\frac{Z}{c_1^3} + \frac{2}{(c_2 - c_1)^3} & -2\frac{1}{(c_2 - c_1)^3} \\ -2\frac{1}{(c_2 - c_1)^3} & -2\frac{Z}{c_2^3} + \frac{2}{(c_2 - c_1)^3} \end{bmatrix}.$$
(8)

Once the roots of equations (7) are found the values of λ can be calculated from the expression below:

$$\lambda = -2\frac{Z}{c_1^3} + \frac{4}{\left(c_2^2 - c_1^2\right)^3} - 2\frac{Z}{c_2^3} + 2.$$
(9)

System (7) can be solved numerically only. However, there is a way of circumventing this lack of closed solution for equations (7) whose solution is necessary to evaluate λ . It consists

of the evaluation of (i) and (ii) for a set of integers p. The solutions given by these values of p are the presumed values of λ for which the system could be integrable. These values of λ form open sets where we can be sure that the system is non-integrable. If the values of λ found using expression (9) are sufficiently far from these presumed values then the theorem guarantees the non-integrability of the FPA being examined. If we solve equations (6) for integers we get the following set of values for the λ for -8 which is sufficient forthis case:

$$\{\cdots, -44, -35, -27, -20, -14, -9, -5, -2, 0, 1\}.$$
 (10)

These values of λ constitute a set of open intervals, say \cdots (-44, -35), (-35, -27), \cdots (-2, 0), (0, 1) where we can be sure the system is not integrable. We recall that the end points of the interval are values of λ where integrability cannot be decided.

The numerical solution of equations (7) consists of 15 pairs of (c_1, c_2) . Evaluating equation (9) we obtain 15 values for λ , but only one of them is real for each value of Z and is listed below.

Ζ	λ
1.01	-9.391 795 19
1.1	-9.32000620
1.5	-9.08758482
1.714 285	-9.00000000
2.0	-8.907 258 16 (helium atom)
3.0	-8.70100689
4.0	-8.58290750
5.0	-8.50480681
10.0	-8.321 775 24
100.0	-8.07050022
1000.0	-8.01596030
:	
$Z \to \infty$	-8

The remaining 14 values are complex numbers with real parts near -8 and -2, which are the limit values of λ as $Z \to \infty$. The limit problem is non-integrable since one of the λ , -8, belongs to one of the non-integrability intervals (-9, -5). Therefore, even the perturbation being small, from the point of view of integrability, it is sufficient that it exists to turn the perturbed Hamiltonian non-integrable. The case $Z = 1.714\,285$ with $\lambda = -9.0$ is also non integrable due to its corresponding complex roots. Numerical simulation gives an integrable looking Poincaré section as the Z = 2 case. Therefore, the two non-integrability point of view. Moreover, we found $\lambda = -8$ for the limit $A \to 0$ for $A/||x_1| - |x_2||$, e.g., A = 0.5, $\lambda = -8.5829$; A = 0.1, $\lambda = -8.2043$; A = 0.01, $\lambda = -8.0445$.

When Z is finite, the real λ are either in the interval (-14, -9) or (-9, -5). Note that for all finite values of Z the real values of the actual λ are sufficiently far from the values -5, -9 and -14. Even calculations with more digits do not change the values such as -9.087 and -8.907. In this case the theorem guarantees the non-integrability of the systems. Therefore, none of these FPA are integrable, even the case Z = 2 with its integrable looking Poincaré section.



Figure 3. Poincaré section (r_2, p_2) , E = -1, $r_1 = 0$ and $p_1 > 0$ for the 1D isoelectronic atom: (*a*) Z = 2, helium atom; (*b*) Z = 3; (*c*) Z = 5; (*d*) Z = 10. Note that the many resonances which appear as Z increases and the non-integrability becomes evident. The helium case seems regular in the whole phase space.

To illustrate this result, figure 3 shows the Poincaré section for some values of the nuclear charge. The islands start to appear for Z = 3 and their stochastic zones overlap spreading irregularity in the phase space. But the inner fixed point (and surrounding iterates on invariant curves) is preserved for all the examples examined. This agrees with the KAM theorem which guarantees the existence of tori (sufficiently far from resonances) even when the problem is non-integrable, that is so-called quasi-integrable systems. That is why there exist adiabatic invariants.

Before examining the cases of the outer/inner electron being replaced by heavier particles, it is important to comment on the numerical resolution of the problem. The solutions of equations (7) were found using the software Maple with 16 digits without previously reducing the equations to rational functions. The software Mathematica gives the same answer. They

agree with the solutions found by Malajovich [12–14]. We also used Maple to directly evaluate equations (7) with the method of the resultant of two polynomials [15]. Therefore, the values presented here have been carefully cross-checked.

3.3. Strange helium atoms (Z = 2)

Before proceeding to calculations we make a canonical change of variables in the Hamiltonian (3) for the FPA to make the result easier to compare with the previous subsection. We take $r'_i = u_i r_i$ and $p'_i = p_i/u_i$, i = 1, 2, where $u_1 = 1/\sqrt{\mu_{12}}$ and $u_2 = 1/\sqrt{\mu_3}$. Now the problem is isotropic in the masses and as before we can write the equations for c_1 and c_2 as

$$c_{1} = \frac{2}{u_{1}c_{1}^{2}} + \frac{2m_{2}}{\left(u_{2}c_{2} + \frac{m_{2}u_{1}}{m_{1} + m_{2}}c_{1}\right)^{2}(m_{1} + m_{2})} + \frac{m_{1}}{\left(u_{2}c_{2} - \frac{m_{1}u_{1}}{m_{1} + m_{2}}c_{1}\right)^{2}(m_{1} + m_{2})}$$

$$c_{2} = \frac{2}{\left(u_{2}c_{2} + \frac{m_{2}u_{1}}{m_{1} + m_{2}}c_{1}\right)^{2}} - \frac{1}{\left(u_{2}c_{2} - \frac{m_{1}u_{1}}{m_{1} + m_{2}}c_{1}\right)^{2}}.$$
(11)

The expression for λ is now:

$$\lambda = \frac{-4}{u_1 c_1^3} - \frac{4u_1^2 m_2^2}{(m_1 + m_2)^2 (u_2 c_2 + \frac{m_2 u_1}{(m_1 + m_2)} c_1)^3} + \frac{2u_1^2 m_1^2}{(m_1 + m_2)^2 (u_2 c_2 - \frac{m_1 u_1}{(m_1 + m_2)} c_1)^3} - \frac{4u_2^2}{(u_2 c_2 + \frac{m_2 u_1}{(m_1 + m_2)} c_1)^3} + \frac{2u_2^2}{(u_2 c_2 - \frac{m_1 u_1}{(m_1 + m_2)} c_1)^3} + 2.$$
(12)

First, we examine the case where the inner electron is substituted by one of the heavier particles: muon, pion, kaon and antiproton. We evaluate c_1 and c_2 , numerically as before, and find the corresponding real values of λ by equation (12). There are again 15 solutions of λ for each case. All the complex values have real part near -2, one of the values shown in the sequence (10) for which the problem could be integrable. Also, this is the value found for the case of the two non-interacting electrons.

The real values of λ for each case are shown in the table below, where $m_3 = 4.002\,602\mu$ and $m_1 = 5.485\,799 \times 10^{-4}\mu$, with $\mu = 931.494\,32$ MeV/ c^2 . We show the electron case at the top of the list to make comparison easier for the reader.

Particle	$m_2(\mu)$	λ	Relevant interval
Electron Muon Pion	5.485799×10^{-4} 0.11342892 0.14983765	-8.905 484 41 -1236.734 498 05 -1618 464 790 53	(-9, -5) (-1274, -1224) (-1652, -1595)
Kaon	0.529 994 32	-5237.978 526 68 -1.031 860 63	(-1032, -1000) (-5252, -5150) (-2, 0)
Antiproton	1.007 295 93	9.143 854 79 -9004.710 370 40 -1.405 213 20 21.417 926 27	$(1, \infty)$ (-9044, -8910) (-2, 0) (1, ∞)

By inspection one can see that the λ are always sufficiently far from the extremes of the open intervals, shown at the right of the table, formed by the solutions of the two equations (6). Of course, they correspond to values of *p* larger than the ones used to obtain the set (10).

The system is not integrable, due to the distance their actual λ are from the extremes of the open intervals of non-integrability given by the solutions of equations (6). Therefore, within

the precision of the masses none of these systems are integrable. This confirms the numerical result given in [8]. The numerical evidence of this fact can be seen in the Poincaré section, shown in figure 2(b), for $m_2/m_e = 30$, where the stable island has become partially chaotic. For values around $m_2/m_e = 35$ this section becomes completely chaotic. Note that all values of the ratio m_2/m_e studied here are much bigger than this value ($m_2/m_e = 200$ for the muon). Poincaré sections calculated for the heavier particle on the outside show that these particles behave like the electron. By this we mean a large regular looking Poincaré section as in the case of the muon shown in figure 2(c). Of course, they have a displaced equilibrium point when compared to the electron case. Therefore, it is interesting to examine the case where the electron is the inner particle. It is sufficient to make the above calculation with the indices 1 and 2 interchanged. For this the result is (showing only real numbers)

Particle	$m_1(\mu)$	λ	Relevant interval
Electron	5.485799×10^{-4}	-8.90548441	(-9, -5)
Muon	0.113 428 92	-2.15707601	(-5, -2)
Pion	0.149 837 65	-2.13425856	(-5, -2)
Kaon	0.529 994 32	-2.05985981	(-5, -2)
Antiproton	1.007 295 93	-2.032 162 66	(-5, -2)

As can be noted by inspection, these values of λ are in the intervals calculated by equations (6) for $p \in (-8, 8)$. These intervals are shown in the right column and it is easy to see that λ are comfortably distant of the extremes where integrability could be possible. Therefore, none of these cases can be integrable.

4. Final comments

We apply the theorem of Morales-Ramis, one of the latest theorems on integrability of Hamiltonian systems, and prove that there is no integrable case for various one-dimensional helium-like atoms described by the frozen planetary approximation. We treat the isoelectronic case for various values of the nuclear charge as well as the strange helium atoms with one electron substituted by a heavier particle: muon, kaon, pion and antiproton either near the α -particle or outside the core $\alpha - e$. The Poincaré sections in some cases give evidence of this non-integrability, but in other cases, such as the helium atom and the strange atoms with the heavier particle on the outside, the systems look integrable in the whole phase space.

Summarizing, we show a computer-aided non-integrability proof of the frozen planetary atom configurations.

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