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INTEGRABILITY OF THE NOSÉ–HOOVER EQUATION

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Abstract. In this work we consider the Nosé–Hoover equation for a one dimensional oscillator

$$\dot{x} = -y - xz, \quad \dot{y} = x, \quad \dot{z} = \alpha(x^2 - 1).$$

It models the interaction of a particle with a heat–bath. We contribute to the understanding of its global dynamics, or more precisely, to the topological structure of its orbits by studying the integrability problem. We prove that $\alpha = 0$ is the only value of the parameter for which the system is integrable, and in this case we provide an explicit expression for its first integrals.

1. Introduction

The *Nosé–Hoover* thermostat is a differential method used in molecular dynamics to keep the temperature around an average. It was first introduced by Nosé [11] and developed further by Hoover [6]. To be more precise in 1985 Nosé considered a physical system of M particles, with the momenta $\mathbf{p} = (p_1, \ldots, p_M)$ and coordinates $\mathbf{q} = (q_1, \ldots, q_M)$ in a fixed volume and a potential energy $V(\mathbf{q})$. He proposed the following model

$$\dot{q}_i = \frac{p_i}{ms^2}, \quad \dot{p}_i = -\frac{\partial V}{\partial q_i}, \quad \dot{s} = p_s/Q, \quad \dot{p}_s = \Big(\sum_{i=1}^{M} \frac{p_i^2}{s^2 m} - gkT\Big)/s,$$

where k is Boltzmann's constant; T is a temperature; g the number of degrees of freedom of the physical system; and Q is a parameter (for more details and generalization see [1]). Subsequently Hoover [6] showed that these equations can be written in a simpler form by transforming to the scaled momentum $\hat{p}_i = p_i/s$ and time scaling $\hat{t} = \int_0^t dt/s$. Thus, after dropping the hat one ends up with the following dynamical system, called *Nosé–Hoover* model

$$\dot{q}_i = \frac{p_i}{m}, \qquad \dot{p}_i = -\frac{\partial V}{\partial q_i} - \xi p_i, \qquad \dot{\xi} = \frac{1}{Q}\Big(\sum_{i=1}^{M} \frac{p_i^2}{s^2 m} - gkT\Big).$$

There is also the associated subsidiary equation for s, namely

$$\frac{ds}{dt} = s\,\xi,$$

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which is not needed to compute the trajectories of the M interacting particles. Since then, this model attracted much attention, see for instance [3, 10, 4, 1, 7, 12, 8], where a number of its mathematical and physical aspects were studied.

In this work we consider the Nosé–Hoover equation in the following form [6]:

$$\dot{x} = -y - xz, \quad \dot{y} = x, \quad \dot{z} = \alpha(x^2 - 1), \tag{1}$$

where $\alpha = 1/Q$ is a real parameter and renamed variables are $x = p$, $y = q$ and $z = \xi$. This system is also called *Nosé–Hoover equation for a one dimensional oscillator*. A number of the dynamic aspects of system (1) have been analysed. In [6] Hoover integrates it numerically for $\alpha = 1$ and $\alpha = 10$. Later Hamilton [4] shows numerically a transition to large–scale irregular dynamics for limited range of α. Periodic orbits for this equation that emerge in bifurcations from heteroclinic cycles have recently been considered by Swinnerton–Dyer and Wagenknecht [12]. We also note, that system (1) is a particular case of the well–known Hide, Skeldon and Acheson dynamo model [5].

Here we further contribute to the understanding of the complexity, or more precisely of the topological structure of the dynamics of system (1) by studying its integrability. For the three dimensional system of differential equations the existence of one first integral reduces the complexity of its dynamics and the existence of two first integrals that are functionally independent solves completely the problem (at least theoretically) of determining its phase portraits. In general for a given differential system it is a difficult problem to determine the existence or non–existence of first integrals. Thus, for proving our main results we shall use the information about invariant algebraic surfaces of this system. This is the basis of the so called Darboux theory of integrability, for more details see Section 2.

We first consider the case in which $\alpha = 0$. We start with the following result.

Theorem 1. *The Nosé–Hoover equation with $\alpha = 0$ is integrable with the following first integrals*

$$H_1 = z \quad \textit{and} \quad H_2 = \begin{cases} (x+y)\exp\big(y/(x+y)\big), & \textit{if } z = 2, \\ \dfrac{(-2x + (-z + \sqrt{z^2-4})y)^{\lambda_2}}{(2x + (z + \sqrt{z^2-4})y)^{\lambda_1}}, & \textit{if } z \neq 2 \end{cases}$$

where

$$\lambda_1 = \frac{1}{2}(-z - \sqrt{z^2-4}) \quad \textit{and} \quad \lambda_2 = \frac{1}{2}(-z + \sqrt{z^2-4}).$$

It is straightforward to verify that H_1 and H_2 in the statement of the theorem are first integrals of the Nosé–Hoover equation when $\alpha = 0$. Therefore the proof of Theorem 1 will be omitted and from now on we consider the case in which $\alpha \in \mathbb{R} \setminus \{0\}$.

The following theorem is the main result of this paper.

Theorem 2. *The following statements hold for the Nosé–Hoover equation with $\alpha \in \mathbb{R} \setminus \{0\}$:*

(a) *It does not admit any polynomial first integral;*
(b) *It does not admit any Darboux polynomial with nonzero cofactor;*
(c) *Its only exponential factors are* e^y *and* $e^{z^2+\alpha(x^2+y^2)}$ *with the cofactors* x *and* $-2\alpha z$*, respectively;*
(d) *It does not admit any Darboux first integral.*

The paper is organised as follows. In Section 2 we introduce some basic definitions and results related to the Darboux theory of integrability that we shall need in order to prove one of our main results. In Section 3 we prove Theorem 2.

2. Preliminary results

During recent years the interest in the study of integrability of differential equations has attracted much attention. Darboux theory of integrability plays a central role in the integrability of the polynomial differential models. It gives a sufficient condition for the integrability inside the family of Darboux functions. More precisely, the significance of this method is that we can compute Darboux first integrals by knowing a sufficient number of algebraic invariant surfaces (the so-called Darboux polynomials) and of the so-called exponential factors. We would like to highlight that it works for real or complex polynomial ordinary differential equations. The study of complex invariant algebraic curves is necessary for obtaining all the real first integrals of a real polynomial differential equation, for more details see [9].

We associate to system (1) the following vector field

$$\mathfrak{X} = (-y - xz)\frac{\partial}{\partial x} + x\frac{\partial}{\partial y} + \alpha(x^2 - 1)\frac{\partial}{\partial z}. \tag{2}$$

Let $U \subset \mathbb{R}^3$ be an open subset. We say that the non–constant function $H\colon U \to \mathbb{R}$ is a *first integral* of the polynomial vector field (2) associated to system (1), if $H(x(t), y(t), z(t)) =$ constant for all values of t for which the solution $(x(t), y(t), z(t))$ of $\mathfrak{X}$ is defined on U. Clearly H is a first integral of $\mathfrak{X}$ on U if and only if $\mathfrak{X}H = 0$ on U. When H is a polynomial we say that H is a *polynomial first integral.*

Let $h = h(x, y, z) \in \mathbb{C}[x, y, z]$ be a non–constant polynomial. We say that $h = 0$ is an *invariant algebraic surface* of the vector field $\mathfrak{X}$ in (2) if it satisfies $\mathfrak{X}h = Kh$, for some polynomial $K = K(x, y, z) \in \mathbb{C}[x, y, z]$, called the *cofactor* of h. Note that K has degree at most 1. The polynomial h is called a *Darboux polynomial*, and we also say that K is the *cofactor* of the Darboux polynomial h. We note that a Darboux polynomial with a zero cofactor is a polynomial first integral.

Let $g, h \in \mathbb{C}[x, y, z]$ be coprime. We say that a non–constant function $E = e^{g/h}$ is an *exponential factor* of the vector field $\mathfrak{X}$ given in (2) if it satisfies $\mathfrak{X}E = LE$, for some polynomial $L = L(x, y, z) \in \mathbb{C}[x, y, z]$, called the *cofactor* of E and having degree at most 1. Note that this relation is equivalent to

$$(-y - xz)\frac{\partial(g/h)}{\partial x} + x\frac{\partial(g/h)}{\partial y} + \alpha(x^2 - 1)\frac{\partial(g/h)}{\partial z} = L. \tag{3}$$

For a geometrical and algebraic meaning of the exponential factors see [2].

A first integral G of system (1) is called of *Darboux type* if it is of the form

$$G = f_1^{\lambda_1} \cdots f_p^{\lambda_p} E_1^{\mu_1} \cdots E_q^{\mu_q}, \tag{4}$$

where $f_1, \ldots, f_p$ are Darboux polynomials, $E_1, \ldots, E_q$ are exponential factors and $\lambda_j, \mu_k \in \mathbb{C}$ for $j = 1, \ldots, p$, $k = 1, \ldots, q$. For more information on the Darboux theory of integrability see, for instance, [9] and the references therein.

For a proof of the next proposition see [2].

Proposition 3. *The following statements hold:*

(a) *If $E = e^{g/h}$ is an exponential factor for the polynomial system* (1) *and h is not a constant polynomial, then $h = 0$ is an invariant algebraic curve.*
(b) *Eventually e^g can be an exponential factor, coming from the multiplicity of the infinite invariant straight line.*

3. Proof of Theorem 2

We separate the proof of Theorem 2 into different propositions.

Proposition 4. *System* (1) *with $\alpha \in \mathbb{R} \setminus \{0\}$ does not admit a polynomial first integral.*

Proof. Let h be a polynomial first integral of system (1). Then it satisfies

$$(-y - xz)\frac{\partial h}{\partial x} + x\frac{\partial h}{\partial y} + \alpha(x^2 - 1)\frac{\partial h}{\partial z} = 0. \tag{5}$$

Without loss of generality we can write

$$h = \sum_{j=1}^{n} h_j(x, y, z), \tag{6}$$

where each $h_j = h_j(x, y, z)$ is a homogeneous polynomial of degree j and we assume that $h_n \neq 0$.

Computing the terms of degree $n + 1$ in (5) we get

$$-xz\frac{\partial h_n}{\partial x} + \alpha x^2 \frac{\partial h_n}{\partial z} = 0. \tag{7}$$

Solving this differential equation we obtain $h_n = h_n[(\alpha x^2 + z^2)/2]$. Since $h_n \neq 0$ is a homogeneous polynomial of degree $n \geq 1$, we conclude that n must be even and $h_n = \alpha_n(\alpha x^2 + z^2)^{n/2}$.

Computing the terms of degree n in (5) we get

$$-y\frac{\partial h_n}{\partial x} + x\frac{\partial h_n}{\partial y} - xz\frac{\partial h_{n-1}}{\partial x} + \alpha x^2 \frac{\partial h_{n-1}}{\partial z} = 0. \tag{8}$$

Solving it with respect to h_{n-1} we obtain

$$h_{n-1} = \pm\alpha_n n \alpha^{1/2} y(\alpha x^2 + z^2)^{n/2-1} \arctan \frac{\alpha^{1/2} x}{|z|} + c_{n-1}[(\alpha x^2 + z^2)/2],$$

where c_{n-1} is a homogeneous polynomial of the variable $\alpha(x^2+z^2)/2$. Since h_{n-1} is a homogeneous polynomial of degree $n-1$ we conclude that

$$\pm\alpha_n n\alpha^{1/2} y(\alpha x^2+z^2)^{n/2-1}=0.$$

Thus, since $\alpha \neq 0$, we get that $\alpha_n = 0$ and consequently $h_n = 0$, which is a contradiction with our assumption. This concludes the proof of the proposition. □

Proposition 5. *System* (1) *with* $\alpha \in \mathbb{R}\setminus\{0\}$ *does not admit any Darboux polynomial with nonzero cofactor.*

Proof. Let h be an irreducible Darboux polynomial of system (1) with nonzero cofactor K, where $K = \alpha_0 + \alpha_1 x + \alpha_2 y + \alpha_3 z$, with $\alpha_i \in \mathbb{C}$ for $i = 0, 1, 2, 3$ not all zero.

Then h satisfies

$$(-y-xz)\frac{\partial h}{\partial x}+x\frac{\partial h}{\partial y}+\alpha(x^2-1)\frac{\partial h}{\partial z}=(\alpha_0+\alpha_1 x+\alpha_2 y+\alpha_3 z)h. \tag{9}$$

It is easy to see by direct computations that h has degree greater or equal to two since system (1) has no Darboux polynomials of degree one with nonzero cofactor. Thus we decompose h as a sum of homogeneous polynomials similarly as in (6), where $n \geq 2$ and $h_n \neq 0$.

Computing the terms of degree $n+1$ in (9) we get

$$-xz\frac{\partial h_n}{\partial x}+\alpha x^2\frac{\partial h_n}{\partial z}=(\alpha_1 x+\alpha_2 y+\alpha_3 z)h_n.$$

Solving this linear differential equation we obtain

$$h_n=\exp\left[\alpha^{-1/2}\alpha_1\arctan\frac{x\alpha^{1/2}}{|z|}+\frac{y\alpha_2[\log(\alpha_2 xyA)-\log(2A^2+2|z|A)]}{A}\right]x^{-\alpha_3}w_n(v),$$

where $A=\sqrt{\alpha x^2+z^2}$ and $w_n(v)$ is a function of the variable $v=(\alpha x^2+z^2)/2$. Since h_n is a homogeneous polynomial of degree n and $\alpha \neq 0$, we conclude that $\alpha_1=\alpha_2=0$ and $\alpha_3=-m$, where m is a nonnegative integer. Thus

$$h_n=c_n x^m(\alpha x^2+z^2)^p, \tag{10}$$

where p and m are nonnegative integers such that $m+2p=n$ and $c_n \in \mathbb{C}\setminus\{0\}$ (since $h_n \neq 0$).

Computing the terms of degree n in (9) we get

$$-y\frac{\partial h_n}{\partial x}+x\frac{\partial h_n}{\partial y}-xz\frac{\partial h_{n-1}}{\partial x}+\alpha x^2\frac{\partial h_{n-1}}{\partial z}=\alpha_0 h_n-mzh_{n-1}. \tag{11}$$

Substituting (10) into equation (11) and solving it with respect to h_{n-1} we obtain

$$h_{n-1}=c_n x^m A^{2p-2}\left[\alpha_0 A\log[2A(A+|z|)]+\alpha_0 A\log\frac{\alpha_0 xA^3}{2}-2py\alpha^{1/2}\arctan\frac{x\alpha^{1/2}}{|z|}\right]$$
$$+c_n m x^{m-1}yA^{2p-2}|z|+x^m w_{n-1}(v),$$

where $w_{n-1}(v)$ is a function of the variable $v=(\alpha x^2+z^2)/2$. Since $\alpha \neq 0$, $c_n \neq 0$ and h_{n-1} is a homogeneous polynomial of degree $n-1$, we get the conditions $p=0$,

$\alpha_0 = 0$, $m-1 \geq 0$ and $2p-2 \geq 0$ which are clearly incompatible. This concludes the proof of the proposition. □

Proposition 6. *The only exponential factors of system* (1) *with* $\alpha \in \mathbb{R} \setminus \{0\}$ *are* e^y *and* $e^{z^2+\alpha(x^2+y^2)}$ *with the cofactors* x *and* $-2\alpha z$, *respectively.*

Proof. It follows from Proposition 3 that we can write $E = e^g$ and g satisfies

$$(12) \qquad (-y - xz)\frac{\partial g}{\partial x} + x\frac{\partial g}{\partial y} + \alpha(x^2 - 1)\frac{\partial g}{\partial z} = (\alpha_0 + \alpha_1 x + \alpha_2 y + \alpha_3 z),$$

where $\alpha_i \in \mathbb{C}$, for $i = 0, 1, 2, 3$ are not all zero.

We first prove that g is a polynomial of degree two. We proceed by contradiction. Assume that g is polynomial of degree $n \geq 3$. We write it as a sum of its homogeneous parts as in equation (6) with h_j replaced by g_j. Without loss of generality we can assume that $g_n \neq 0$. Then since the right–hand side of equation (12) has degree at most one, computing the terms of degree $n+1$ in equation (12) we get

$$-xz\frac{\partial g_n}{\partial x} + \alpha x^2 \frac{\partial g_n}{\partial z} = 0,$$

which is equation (7) replacing h_n by g_n. Then the arguments used in the proof of Proposition 4 imply that n must be even and g_n must be of the form $g_n = \alpha_n(\alpha x^2 + z^2)^{n/2}$ with $\alpha_n \in \mathbb{C} \setminus \{0\}$.

Now computing the terms of degree $n \geq 3$ in (12) and taking into account that the right–hand side of (12) has degree one, we get equation

$$-y\frac{\partial g_n}{\partial x} + x\frac{\partial g_n}{\partial y} - xz\frac{\partial g_{n-1}}{\partial x} + \alpha x^2 \frac{\partial g_{n-1}}{\partial z} = 0,$$

which is equation (8) with h_n replaced by g_n and h_{n-1} replaced by g_{n-1}. The arguments used in the proof of Proposition 4 imply that $g_n = 0$. Then we have that $g_n = 0$ for $n \geq 3$, and thus, g is a polynomial of degree at most two satisfying (12). Solving now (12) we get that g can be either y with cofactor x or $z^2+\alpha(x^2+y^2)$ with cofactor $-2\alpha z$ and the proposition follows. □

3.1. **Proof of Theorem 2.** Statements (a), (b) and (c) in the theorem follow directly from Propositions 4, 5 and 6, respectively. In what follows we prove the statement (d) by contradiction. Assume that G is a first integral of Darboux type. Then in view of its definition in (4) and taking into account Propositions 4, 5 and 6, G must be of the form

$$G = e^{\mu_1 x + \mu_2[z^2+\alpha(x^2+y^2)]}, \quad \text{with} \quad \mu_1, \mu_2 \in \mathbb{C}.$$

Since G is a first integral it must satisfy $\mathfrak{X}G = 0$, that is,

$$\begin{aligned}\mathfrak{X}G &= (-y - xz)\frac{\partial G}{\partial x} + x\frac{\partial G}{\partial y} + \alpha(x^2 - 1)\frac{\partial G}{\partial z} \\ &= (\mu_1 x - 2\mu_2 \alpha z)G = 0.\end{aligned}$$

Hence,

$$\mu_1 x - 2\mu_2 \alpha z = 0,$$

and since $\alpha \neq 0$, this implies $\mu_1 = \mu_2 = 0$. Then $G =$ constant, in contradiction with the fact that G was a first integral. This concludes the proof of the theorem.

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