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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 [1] and developed further by Hoover [2]. 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

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

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 [3]). Subsequently Hoover [2] showed that these equations can be

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