

## HOMOTOPY ANALYSIS OF EXPLICIT SERIES SOLUTIONS IN A MODIFIED NOSÉ-HOOVER OSCILLATOR

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**Abstract.** In light of recent advancements in the literature concerning the Homotopy Analysis Method (HAM), this paper introduces a stepwise homotopy analysis methodology. This approach is employed to derive explicit series solutions for a generalized Nosé-Hoover oscillator. Using an optimized homotopy analysis strategy, the computational efficiency of HAM is enhanced through small step intervals, significantly expediting the convergence of series solutions over an extended duration. Comparative analyses between analytical and numerical results are illustrated. The fluctuation in amplitude of the approximate analytical solutions, with respect to the control parameters of the system, is used to generate density plots. These plots serve to highlight additional dynamic features of the oscillator.

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### 1. Introduction

A new paradigm in the study of thermodynamics has been achieved with the introduction, by Shiuchi Nosé in 1984, of a particular set of differential equations (please see [1] and references therein). Different aspects of the study of the Nosé's oscillator

throughout the years, namely its meaning and connections with other fields, can be found in [2–6]. As a consequence of the Nosé’s equations, in 1986, Hoover and his collaborators, Posch and Vesely, obtained the Nosé-Hoover oscillator corresponding to the following equations of motion [7]

$$\frac{dx}{dt} = y; \quad \frac{dy}{dt} = -x - yz; \quad \frac{dz}{dt} = \alpha (y^2 - 1), \quad (1)$$

where  $x$  represents the oscillator coordinate,  $y$  represents momentum and  $z$  represents the friction coefficient, dynamical variables of a one-dimensional harmonic oscillator. As the role of the friction coefficient  $z$  is to maintain the average temperature equal to 1,  $\alpha$  is a positive coupling control parameter. The explicit series solutions reported in the present paper consider a generalized Nosé-Hoover oscillator [8], more specifically the two-parameter set of three nonlinear ordinary differential equations given by

$$\frac{dx}{dt} = y; \quad \frac{dy}{dt} = -x - yz; \quad \frac{dz}{dt} = \alpha (y^2 - 1 - \varepsilon z). \quad (2)$$

This system differs from the original form of the Nosé-Hoover oscillator (1) by the small dissipative term added to the energizing-dapping variable  $z$ , a term that includes the parameter  $\varepsilon$ . In this article, the variation of the approximate analytical solutions of (2) with  $\alpha$  and  $\varepsilon$  will be considered.

Given the importance of the Nosé-Hoover oscillator, several numerical algorithms for approximating solutions have been used. Nevertheless, we are only able to study the dynamics at discrete points. In this context, there are no analytical expressions for the solutions, preventing the examination of the system’s behavior from a continuous perspective. Exact solutions for nonlinear equations are generally challenging to obtain, leading to the widespread use of perturbation techniques, transforming nonlinear problems into mostly linear sub-problems. Despite their success, these methods are constrained by the necessity of small physical parameters and limited flexibility, making them primarily applicable to weakly nonlinear problems. Non-perturbation methods, like Lyapunov’s Artificial Small Parameter Method and the Adomian Decomposition Method [9], offer alternatives but come with limitations, such as the lack of freedom to choose nonlinear operators and uncertainty regarding convergence. Consequently, both perturbation and traditional non-perturbation methods are typically valid for weakly nonlinear problems. Recognizing these limitations, there is a call for the development of a new analytic approximation methodology. The Homotopy Analysis Method (HAM), pioneered by Liao (see, for instance, [10–15]), has precisely the following *three essential advantages*, emerging as a powerful analytic technique for obtaining convergent series solutions to strongly nonlinear problems: (i) independence from small/large physical parameters, (ii) freedom to choose equation types and solution expressions for high-order approximations, and (iii) a reliable distinguished mechanism to ensure the convergence of approximation series solutions, using an artificial convergence control parameter.

The HAM surpasses limitations of traditional methods like Lyapunov's Artificial Small Parameter Method, the Adomian Decomposition Method, and the Homotopy Perturbation Method.

This paper introduces the Step Homotopy Analysis Method (SHAM), a modification of the Homotopy Analysis Method (HAM) outlined in [13]. SHAM is applied to derive approximate analytical solutions for the perturbed Nosé-Hoover model. In this approach, HAM is treated as an algorithm within a specific sequence of small intervals, extending the homotopy analysis technique to achieve accurate approximate solutions, especially applicable during a high value of time  $t$ . Upon implementation, it becomes evident that solutions obtained using the conventional one-time step HAM are valid only for a brief time interval. In contrast, solutions derived through SHAM remain valid for an extended time, accommodating the necessary duration to meet our requirements.

## 2. A concise description of HAM

Let us consider a system of  $r$  ordinary differential equations, and their respective initial conditions, given by

$$\dot{x}_i = f_i(t, x_1, \dots, x_r), \quad x_i(t_0) = x_{i,0}, \quad i = 1, 2, \dots, r. \quad (3)$$

To start with, according to HAM [13], each equation of the system (3) is written in the form  $\mathcal{N}_i[x_1(t), x_2(t), \dots, x_r(t)] = 0$ ,  $i = 1, 2, \dots, r$ , where  $\mathcal{N}_i$  are nonlinear operators,  $x_i(t)$  are unknown functions, and  $t$  denotes the independent variable. From a generalization of the traditional homotopy method, it has been established that the so-called *zero<sup>th</sup>-order deformation equation* is given by

$$(1 - q) \mathcal{L}[\phi_i(t; q) - x_{i,0}(t)] = q h \mathcal{N}_i[\phi_1(t; q), \dots, \phi_r(t; q)], \quad (4)$$

where  $q \in [0, 1]$  is an embedding parameter,  $\mathcal{L}$  is an auxiliary linear operator,  $\phi_i(t; q)$  are unknown functions,  $x_{i,0}(t)$  are initial guesses, and  $h$  is a non-zero auxiliary artificial parameter. In the context of HAM, there is great freedom to choose auxiliary entities such as  $\mathcal{L}$ ,  $h$  and base functions for the representation of the solution  $x_i(t)$ . Notice that, when  $q = 0$  and  $q = 1$ , both  $\phi_i(t; 0) = x_{i,0}(t)$  and  $\phi_i(t; 1) = x_i(t)$  hold. According to (4), as  $q$  increases from 0 to 1, the function  $\phi_i(t; q)$  varies from the initial guess  $x_{i,0}(t_0) = x_i(t_0)$ , at  $t = t_0$ , to the solution  $x_i(t)$ . The expansion of  $\phi_i(t; q)$  in the Taylor series with respect to  $q$ , is given by

$$\phi_i(t; q) = x_{i,0}(t) + \sum_{m=1}^{+\infty} x_{i,m}(t) q^m, \quad \text{where } x_{i,m}(t) = \frac{1}{m!} \left. \frac{\partial^m \phi_i(t; q)}{\partial q^m} \right|_{q=0}. \quad (5)$$

When the auxiliary linear operators, the base functions, and the auxiliary parameter  $h$ , are properly chosen, the series (5) converges at  $q = 1$  and

$$x_i(t) = \phi_i(t; 1) = x_{i,0}(t) + \sum_{m=1}^{+\infty} x_{i,m}(t), \quad i = 1, 2, \dots, r,$$

which are the solutions of the original nonlinear equations. Taking the  $m^{\text{th}}$ -order homotopy-derivative of the  $zero^{\text{th}}$ -order Eqs. (4), and using the corresponding properties, we obtain the  $m^{\text{th}}$ -order deformation equations

$$\mathcal{L} [x_{i,m}(t) - \chi_m x_{i,m-1}(t)] = h R_{i,m} [x_{1,m-1}(t), \dots, x_{r,m-1}(t)], \quad i = 1, 2, \dots, r, \quad (6)$$

$$\text{where: } R_{i,m} [x_{1,m-1}(t), \dots, x_{r,m-1}(t)] = \frac{1}{(m-1)!} \frac{\partial^{m-1} N_i [\phi_1(t; q), \dots, \phi_r(t; q)]}{\partial q^{m-1}} \Big|_{q=0},$$

$\chi_m = \begin{cases} 0, & m \leq 1 \\ 1, & m > 1 \end{cases}$  and  $\mathcal{L}$  is the time differentiation operator. Solutions of linear  $m^{\text{th}}$ -order deformation equations (6), satisfying the initial conditions, for all  $m \geq 1$ , are given by

$$x_{i,m}(t) = \chi_m x_{i,m-1}(t) + h \int_0^t R_{i,m} [x_{1,m-1}(\tau), \dots, x_{r,m-1}(\tau)] d\tau.$$

Truncating the homotopy series solutions  $x_i(t) = x_{i,0}(t) + \sum_{m=1}^{+\infty} x_{i,m}(t)$ , at the  $M^{\text{th}}$  step, we obtain the  $M^{\text{th}}$ -order approximate solutions in the form

$$x_i^{(M)}(t) = x_{i,0}(t) + \sum_{m=1}^M x_{i,m}(t), \quad \text{where } i = 1, 2, 3, \dots, r.$$

Given the specificities of different nonlinear problems, different orders of approximation can be used. With the described procedure, the HAM converts a complicated nonlinear problem into simpler linear sub-problems. For some strongly nonlinear problems, this described one-time step HAM scheme is only accurate for a short value of  $t$ . As a consequence, it is appropriate to use the previously mentioned Step Homotopy Analysis Method (SHAM). As already pointed out, with the SHAM approach, HAM is treated as an algorithm in each of the successive time step intervals of small amplitude. This computational scheme generalizes the homotopy analysis approach for finding accurate approximate solutions for a nonlinear problem, in terms of a convergent series with easily computable components, valid for a high value of  $t = T$ . More precisely, in the context of SHAM, let  $[0, T]$  be the interval over which we want to find the solution of the initial value problem (3). We start by assuming that the interval  $[0, T]$  is divided into  $n$ -subintervals of equal length  $\Delta t$ ,  $[t_0, t_1]$ ,  $[t_1, t_2]$ ,  $[t_2, t_3]$ , ...,  $[t_{n-2}, t_{n-1}]$ ,  $[t_{n-1}, t_n]$ , with  $t_0 = 0$  and  $t_n = T$ , as illustrated in Figure 1. Each subinterval has the form  $[t_{j-1}, t_j]$ ,  $j = 1, 2, 3, \dots, n$ . Let  $t^* = t_{j-1}$  be the initial value of each

subinterval. The  $M^{th}$ -order approximate solutions of the given system (3), in each subinterval  $[t_{j-1}, t_j]$ ,  $j = 1, 2, 3, \dots, n$ , will have the form

$$x_{i,j}^{(M)}(t) = x_{i,j,0}(t) + \sum_{m=1}^M x_{i,j,m}(t-t^*), \quad i = 1, 2, \dots, r, \quad j = 1, 2, 3, \dots, n. \quad (7)$$

For the initial value of each subinterval,  $t = t^*$ , the initial values of the dynamical variables  $x_{i,j,0}$ ,  $i = 1, 2, \dots, r$ ,  $j = 1, 2, 3, \dots, n$ , satisfy the family of solutions (7), since for all  $m \geq 1$  we conveniently obtain the terms  $x_{i,j,m}(0) = 0$ . In the beginning of the procedure, only the initial data at  $t = t^* = 0$  is known for  $x_{i,j}^{(M)}(t)$ ,  $i = 1, 2, \dots, r$ ,  $j = 1, 2, 3, \dots, n$ . The initial conditions will be changed at each subinterval. In particular, the corresponding initial values at  $t^* = t_{j-1}$ , for  $j = 2, 3, \dots, n$ , of each one of the following step intervals, is obtained by using the previous approximate solutions computed at the previous step, thus ensuring continuity of solutions.



Fig. 1. Interval  $[0, T]$  divided into a sequence of  $n$ -subintervals,  $[t_{j-1}, t_j]$ ,  $j = 1, 2, 3, \dots, n$ , of equal length  $\Delta t$

### 3. The step homotopy analysis technique and the analytic solutions

The analytical approach of HAM [13] will be used in a sequence of intervals, giving rise to the mentioned Step Homotopy Analysis Method (SHAM). In the following section, we outline the description of SHAM applied to the modified Nosé-Hoover model (2).

#### 3.1. Explicit series solutions

Based on the primary definitions of the HAM, we are able to obtain explicit approximation series solutions for the state variables  $x$ ,  $y$ , and  $z$  of the generalized Nosé-Hoover model (2). Let us consider our approximations  $x(t)$ ,  $y(t)$  and  $z(t)$  that are defined by constant functions taking the initial condition values such that  $x_0(t) = x_0$ ,  $y_0(t) = y_0$ , and  $z_0(t) = z_0$ . For our present analysis, we set the following values for the initial conditions  $x_0 = 0.9209$ ,  $y_0 = -0.1560$  and  $z_0 = 0.9179$ . In the context of HAM, there is freedom to choose auxiliary linear operators, and we are going to consider

$$\mathcal{L}[\phi_1(t; q)] = \frac{\partial \phi_1(t; q)}{\partial t}, \quad \mathcal{L}[\phi_2(t; q)] = \frac{\partial \phi_2(t; q)}{\partial t} \quad \text{and} \quad \mathcal{L}[\phi_3(t; q)] = \frac{\partial \phi_3(t; q)}{\partial t},$$

with the property  $\mathcal{L}(c_i) = 0$ , where  $c_i$  ( $i = 1, 2, 3$ ) are integral constants. The non-linear operators for the Nosé-Hoover oscillator (2) are defined as follows:

$$\begin{aligned}\mathcal{N}_1[\phi_1(t; q), \phi_2(t; q), \phi_3(t; q)] &= \frac{\partial \phi_1(t; q)}{\partial t} - \phi_2(t; q), \\ \mathcal{N}_2[\phi_1(t; q), \phi_2(t; q), \phi_3(t; q)] &= \frac{\partial \phi_2(t; q)}{\partial t} + \phi_1(t; q) + \phi_2(t; q)\phi_3(t; q), \\ \mathcal{N}_3[\phi_1(t; q), \phi_2(t; q), \phi_3(t; q)] &= \frac{\partial \phi_3(t; q)}{\partial t} - \alpha\phi_2^2(t; q) + \alpha + \alpha\varepsilon\phi_3(t; q).\end{aligned}$$

The zero<sup>th</sup>-order deformation equations assume the form

$$\begin{aligned}(1-q)\mathcal{L}[\phi_1(t; q) - x_0(t)] &= qh\mathcal{N}_1[\phi_1(t; q), \phi_2(t; q), \phi_3(t; q)], \\ (1-q)\mathcal{L}[\phi_2(t; q) - y_0(t)] &= qh\mathcal{N}_2[\phi_1(t; q), \phi_2(t; q), \phi_3(t; q)], \\ (1-q)\mathcal{L}[\phi_3(t; q) - z_0(t)] &= qh\mathcal{N}_3[\phi_1(t; q), \phi_2(t; q), \phi_3(t; q)],\end{aligned}\quad (8)$$

with initial conditions  $\phi_1(0; q) = 0.9209$ ,  $\phi_2(0; q) = -0.1560$  and  $\phi_3(0; q) = 0.9179$ . Given the zero<sup>th</sup>-order equations (8), their solutions are:

$$\begin{aligned}\text{for } q = 0 &\rightarrow \phi_1(t; 0) = x_0(t), \phi_2(t; 0) = y_0(t), \text{ and } \phi_3(t; 0) = z_0(t), \\ \text{for } q = 1 &\rightarrow \phi_1(t; 1) = x(t), \phi_2(t; 1) = y(t), \text{ and } \phi_3(t; 1) = z(t).\end{aligned}\quad (9)$$

By increasing  $q$  from 0 to 1, the functions  $\phi_i(t; q)$  ( $i = 1, 2, 3$ ) vary from  $x_0(t)$ ,  $y_0(t)$  and  $z_0(t)$  to  $x(t)$ ,  $y(t)$  and  $z(t)$ , respectively. Expanding each of the functions  $\phi_i(t; q)$  ( $i = 1, 2, 3$ ) in the Taylor series, with respect to  $q$ , we obtain the homotopy series

$$\begin{aligned}\phi_1(t; q) &= x_0(t) + \sum_{m=1}^{+\infty} x_m(t)q^m, \quad \phi_2(t; q) = y_0(t) + \sum_{m=1}^{+\infty} y_m(t)q^m, \\ \phi_3(t; q) &= z_0(t) + \sum_{m=1}^{+\infty} z_m(t)q^m, \quad \text{where}\end{aligned}\quad (10)$$

$$x_m(t) = \frac{1}{m!} \left. \frac{\partial^m \phi_1(t; q)}{\partial q^m} \right|_{q=0}, \quad y_m(t) = \frac{1}{m!} \left. \frac{\partial^m \phi_2(t; q)}{\partial q^m} \right|_{q=0}, \quad z_m(t) = \frac{1}{m!} \left. \frac{\partial^m \phi_3(t; q)}{\partial q^m} \right|_{q=0}.\quad (11)$$

The auxiliary parameter  $h$  is chosen properly to ensure the convergence, of all series, for  $q = 1$ . From Eqs. (9)-(11), we obtain the homotopy series solutions

$$x(t) = x_0(t) + \sum_{m=1}^{+\infty} x_m(t), \quad y(t) = y_0(t) + \sum_{m=1}^{+\infty} y_m(t), \quad \text{and } z(t) = z_0(t) + \sum_{m=1}^{+\infty} z_m(t).\quad (12)$$

Now, we differentiate the zero<sup>th</sup>-order Eqs. (8)  $m$  times using the following properties that, for illustrative purposes, are applied to arbitrary dynamical variables  $x_i$  ( $i = 1, 2, 3$ ). The terms  $x_m$ ,  $y_m$  and  $z_m$  of the Nosé-Hoover dynamical variables correspond to the terms of these dynamical variables  $x_{1,m}$ ,  $x_{2,m}$  and  $x_{3,m}$ , used to state the

selected algebraic properties of the HAM methodology, that is,  $x_m = x_{1,m}$ ,  $y_m = x_{2,m}$ , and  $z_m = x_{1,m}$ .

$$\begin{aligned} \mathcal{D}_m(\phi_i) &= x_{i,m}, \quad \mathcal{D}_m(q^k \phi_i) = \mathcal{D}_{m-k}(\phi_i) = \begin{cases} x_{i,m-k}, & 0 \leq k \leq m, \\ 0, & \text{otherwise} \end{cases} \\ \mathcal{D}_m(\phi_1^2) &= \sum_{k=0}^m x_{i,m-k} x_{i,k}, \quad \mathcal{D}_m(\phi_i \psi_i) = \sum_{k=0}^m \mathcal{D}_k(\phi_i) \mathcal{D}_{m-k}(\psi_i) = \sum_{k=0}^m x_{i,k} y_{i,m-k}, \end{aligned}$$

where  $\mathcal{D}_m$  stands for the  $m^{\text{th}}$ -order derivative with respect to the homotopy parameter  $q$ . As a consequence, we obtain the  $m^{\text{th}}$ -order deformation equations

$$\begin{aligned} \mathcal{L}[x_m(t) - \chi_m x_{m-1}(t)] &= h R_{1,m}[\vec{u}_{m-1}(t)], \\ \mathcal{L}[y_m(t) - \chi_m y_{m-1}(t)] &= h R_{2,m}[\vec{u}_{m-1}(t)], \\ \mathcal{L}[z_m(t) - \chi_m z_{m-1}(t)] &= h R_{3,m}[\vec{u}_{m-1}(t)], \end{aligned} \quad (13)$$

for which  $x_m(0) = 0$ ,  $y_m(0) = 0$ ,  $z_m(0) = 0$ , where

$$\chi_m = \begin{cases} 0, & \text{for } m \leq 1 \\ 1, & \text{for } m > 1 \end{cases}, \quad \vec{u}_{m-1}(t) = (x_{m-1}(t), y_{m-1}(t), z_{m-1}(t)), \quad m = 1, 2, 3, \dots$$

$$\begin{aligned} R_1[\vec{u}_{m-1}] &= \frac{dx_{m-1}(t)}{dt} - y_{m-1}(t), \\ R_2[\vec{u}_{m-1}] &= \frac{dy_{m-1}(t)}{dt} + x_{m-1} + \sum_{k=0}^{m-1} y_{m-1-k}(t) z_k(t) \\ \text{and } R_3[\vec{u}_{m-1}] &= \frac{dz_{m-1}(t)}{dt} - \alpha \sum_{k=0}^{m-1} y_{m-k}(t) y_k(t) + (1 - \chi_m) \alpha + \alpha \varepsilon z_{m-1}(t). \end{aligned}$$

Solutions of the linear  $m^{\text{th}}$ -order deformation equations (13), satisfying the initial conditions  $x_m(0) = 0$ ,  $y_m(0) = 0$ ,  $z_m(0) = 0$  for all  $m \geq 1$ , are given by

$$\begin{aligned} x_m(t) &= \chi_m x_{m-1}(t) + h \int_0^t R_{1,m}[\vec{u}_{m-1}(t)] d\tau, \quad y_m(t) = \chi_m y_{m-1}(t) + h \int_0^t R_{2,m}[\vec{u}_{m-1}(t)] d\tau \\ \text{and } z_m(t) &= \chi_m z_{m-1}(t) + h \int_0^t R_{3,m}[\vec{u}_{m-1}(t)] d\tau. \end{aligned} \quad (14)$$

For the computation of each term of order  $m = 1, 2, 3, \dots$ , only the respective term of order  $m - 1$  is needed. Truncating the homotopy series (12) at the  $M^{\text{th}}$  step, we obtain the  $M^{\text{th}}$ -order approximate solutions in the form

$$x^{(M)}(t) = x_0(t) + \sum_{m=1}^M x_m(t), \quad y^{(M)}(t) = y_0(t) + \sum_{m=1}^M y_m(t) \quad \text{and} \quad z^{(M)}(t) = z_0(t) + \sum_{m=1}^M z_m(t), \quad (15)$$

where  $M = 1$  corresponds to the initial conditions,  $M = 2$  corresponds to:

$$\begin{aligned} x^{(2)}(t) &= 0.9209 + 0.312ht + h(0.156ht - 0.38885ht^2)t \\ y^{(2)}(t) &= -0.156 + 1.55542ht + h(0.77770ht \\ &\quad + 0.43492ht^2 - 0.076101ht^2\alpha - 0.07159ht^2\alpha\varepsilon) \\ z^{(2)}(t) &= 0.9179 + 2ht(0.97566\alpha + 0.9179\alpha\varepsilon) + h(0.97566ht\alpha \\ &\quad + 0.12132ht^2\alpha + 0.9179ht\alpha\varepsilon + 0.48783ht^2\alpha^2\varepsilon + 0.45895ht^2\alpha^2\varepsilon^2), \end{aligned}$$

and, similarly, the aforementioned procedure applies to the remaining terms in the series solutions (15). In order to obtain approximations to solutions for large values of  $t$ , we use the SHAM, which corresponds to the application of the HAM on a sequence of intervals with the time step  $\Delta t$ . For illustrative purposes, let us consider the  $9^{th}$ -order approximations

$$x^{(9)}(t) = x_0(t) + \sum_{m=1}^9 x_m(t), \quad y^{(9)}(t) = y_0(t) + \sum_{m=1}^9 y_m(t) \quad \text{and} \quad z^{(9)}(t) = z_0(t) + \sum_{m=1}^9 z_m(t). \quad (16)$$

Notice that we can use approximations of any desired order that serves our particular needs. Using SHAM, the  $9^{th}$ -order approximate solutions of the given system (2) in each subinterval  $[t_{j-1}, t_j]$ ,  $j = 1, 2, 3, \dots, n$ , have the form

$$\begin{aligned} x^{(9)}(t) &= x(t^*) + \sum_{m=1}^9 x_m(t - t^*), \quad y^{(9)}(t) = y(t^*) + \sum_{m=1}^9 y_m(t - t^*) \quad \text{and} \\ z^{(9)}(t) &= z(t^*) + \sum_{m=1}^9 z_m(t - t^*). \end{aligned} \quad (17)$$

By determining the variables  $x(t)$ ,  $y(t)$  and  $z(t)$  for  $t = t^* = 0$ , the corresponding initial values for the subsequent step intervals at  $t^* = t_{j-1}$ , where  $j = 2, 3, \dots, n$ , are computed using the previously approximated solutions obtained at the preceding step. This ensures the smooth progression of solutions. The homotopy terms are dependent on both the physical variable  $t$  and the convergence control parameter  $h$ . How can an appropriate value for the convergence control parameter  $h$  be identified to achieve a convergent series solution? Moreover, is there a way to expedite the convergence of the series? These queries form the focus of the subsequent section.

### 3.2. Interval of convergence and optimal value for $h$

In this section, we describe an optimization technique that enables us to achieve two objectives: (i) identify all values of the control parameter  $h$  for which the series converges to the exact solution, and (ii) tackle the challenge of selecting the optimal  $h$ , ensuring the fastest convergence of the series (for details, please see [13]).

Let us consider  $k + 1$  homotopy terms  $x_0(t), x_1(t), x_2(t), \dots, x_k(t)$  of an homotopy series  $x(t) = x_0(t) + \sum_{m=1}^{+\infty} x_m(t)$ . According to what is stated in [13] and considering

an interval of time  $\Omega$ , the ratio  $\beta = \frac{\int_{\Omega} [x_k(t)]^2 dt}{\int_{\Omega} [x_{k-1}(t)]^2 dt}$  with  $\frac{\int_{\Omega} [x_k(t)]^2 dt}{\int_{\Omega} [x_{k-1}(t)]^2 dt} < 1$  and

$\frac{d\beta}{dh} = 0$ , offers a convenient way to evaluate the convergence control parameter  $h$  (and similarly for variables  $y$  and  $z$ ). For a given order of approximation, the  $\beta$  versus  $h$  curves not only define the effective region for the convergence control parameter but also identify the optimal  $h$  value corresponding to the absolute minimum of  $\beta$ . Notably, reaching a minimum is not essential for HAM convergence; the critical factor is choosing a value that makes the ratio  $\beta$  less than unity. By plotting  $\beta$  against  $h$ , the convergence interval and the optimal value for the parameter  $h$  can be simultaneously determined. At the  $M = 9$  order of approximation, Figure 2 (left column) displays the curves of ratio  $\beta$  versus  $h$  for  $x(t)$ ,  $y(t)$  and  $z(t)$ . Table 1 presents the corresponding convergence intervals of  $h$  and their optimal values, denoted as  $h^*$ .

Using the ratio  $\beta$ , we can efficiently determine the exact convergence interval and optimal  $h$  value, providing a key advantage in studying HAM convergence. In the right column of Figure 2, the SHAM analytical solutions for  $x$ ,  $y$ , and  $z$  are compared with numerical results, using the optimal values from Table 1.

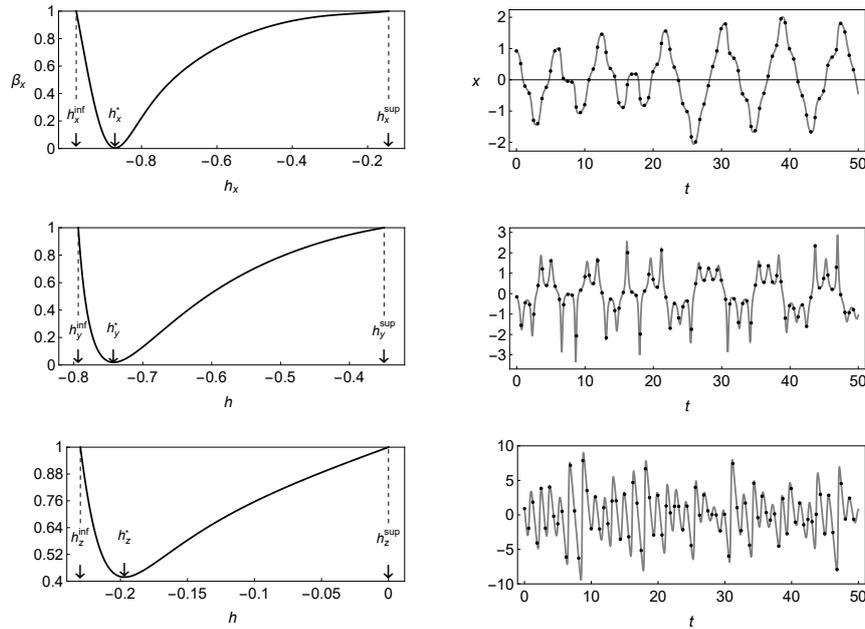


Fig. 2. Left column – The curves of ratios  $\beta_x$ ,  $\beta_y$  and  $\beta_z$  versus  $h_x$ ,  $h_y$  and  $h_z$ , corresponding to a  $9^{th}$ -order approximation of solutions ( $k = M = 9$ ). The optimum values of  $h$ ,  $h^*$ , give rise to the minimum values of the curves  $\beta$ . Right column – Comparison of the approximate SHAM analytical solutions (17) of  $x(t)$ ,  $y(t)$  and  $z(t)$  (solid lines) with the respective numerical solutions (dotted lines), considering  $t \in [0, 50]$ . In all situations,  $\alpha = 11$  and  $\varepsilon = 0.00002$

Table 1. Intervals of convergence of  $h$  and the respective optimum values  $h^*$ , corresponding to the dynamical regimes presented in Figure 2

$\beta$ -Curves	Convergence intervals	Convergence optimal values of $h$
$\beta_x$	$-0.97318 < h_x < -0.14430$	$h_x^* = -0.86987$
$\beta_y$	$-0.79358 < h_y < -0.34984$	$h_y^* = -0.74239$
$\beta_z$	$-0.22990 < h_z < 0$	$h_z^* = -0.19696$

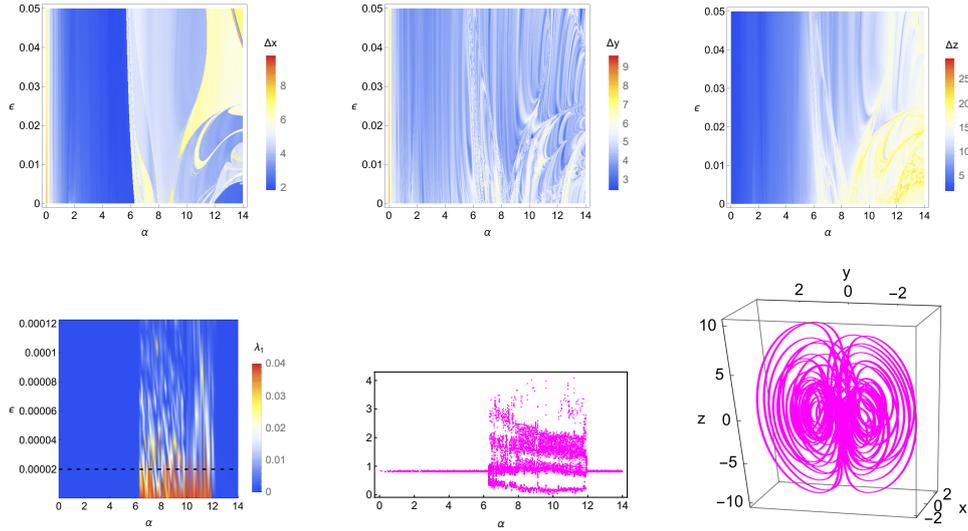


Fig. 3. Upper panel – Density plots representing the variation of the maximum amplitude of  $x$ ,  $y$  and  $z$  time series. Lower panel – Density plot depicting the MLE variation; Bifurcation diagram displaying the long-term behavior of the system (2) for  $\varepsilon = 0.00002$  and  $\alpha \in [0, 14]$ ; Nosé-Hoover attractor for  $\varepsilon = 0.00002$  and  $\alpha = 11$

Additionally, Figure 3 illustrates the variation of amplitude for the dynamical variables. Notably, for  $x$  and  $z$ , the amplitude variation is particularly diverse, associated with positive values of the Maximum Lyapunov Exponent (MLE),  $\lambda_1$ , indicating chaotic behavior. Specifically, for  $\alpha = 11$  and  $\varepsilon = 0.00002$ , we obtain  $\lambda_1 = 0.033350$ . A density plot depicting the MLE variation is shown, and the bifurcation diagram represents the long-term behavior of the system (2) with  $\varepsilon = 0.00002$  and  $\alpha \in [0, 14]$  (as indicated by the dashed line in the MLE density plot). Figure 3 also presents the Nosé-Hoover attractor for  $\alpha = 11$  and  $\varepsilon = 0.00002$ . For solutions in the chaotic region, and for a larger value of  $t$ , namely  $t = T = 10^6$ , the same analysis has been performed, and the same qualitative behavior has been obtained.

#### 4. Conclusion

This paper introduces the Step Homotopy Analysis Method (SHAM), which is a modification of the Homotopy Analysis Method (HAM), for obtaining approximate analytical solutions to the perturbed Nosé-Hoover model. HAM is treated as an algo-

rithm in a sequence of small intervals, generalizing the one-step homotopy analysis for accurate solutions valid at a high value of  $t$ . Solutions obtained with one-time step HAM are limited to a short time interval, while SHAM extends validity for  $t$  as necessary. The homotopy analysis approach is independent of physical parameters, and its terms depend on both  $t$  and the convergence control parameter  $h$ . This parameter  $h$  can be chosen freely within a determined interval of convergence. For practical purposes,  $h$  is crucial in HAM, allowing accurate approximations with minimal homotopy terms. This sets HAM apart from other perturbation-like techniques. This study demonstrates the potential of HAM for solving highly nonlinear problems, showcasing an integrated approach that combines numerical evidence and theoretical reasoning within the theory of dynamical systems, enhancing our understanding of nonlinear models, especially in a physical context.

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## References

- [1] Nosé, S. (1984). A molecular dynamics method for simulations in the canonical ensemble. *Molecular Physics*, 52, 2, 255-268.
- [2] Sprott, J.C., Hoover, W.G., & Hoover, C.G. (2014). Heat conduction and the lack thereof, in time-reversible dynamical systems: Generalized Nosé-Hoover oscillators with a temperature gradient. *Physical Review E*, 89, 042914.
- [3] Sprott, J.C. (2020). Variants of the Nosé-Hoover oscillator. *The European Physical Journal, Special Topics*, 229, 963-971.
- [4] Shijian, C., Gehang, Z., Zenghui, W., & Zengqiang, C. (2022). Global structures of clew-shaped conservative chaotic flows in a class of 3D one-thermostat systems. *Chaos, Solitons and Fractals*, 154, 111687.
- [5] Fukuda, I. (2016). Coupled Nosé-Hoover lattice: A set of the Nosé-Hoover equations with different temperatures. *Physics Letters A*, 380, 33, 2465-2474.
- [6] Wang, L., & Yang, X. (2018). Global analysis of a generalized Nosé-Hoover oscillator. *Journal of Mathematical Analysis and Applications*, 464, 1, 370-379.
- [7] Posch, H.A., Hoover, W.G., & Vesely, F.G. (1986). Canonical dynamics of the Nosé oscillator: Stability, order, and chaos. *Physical Review A*, 33, 4253.
- [8] Han, Q., Deng, B., & Yang, X-S. (2022). The existence of  $\omega$ -limit set for a modified Nosé-Hoover oscillator. *Discrete and Continuous Dynamical Systems Series B*, 27, 7275-7300.
- [9] Zhang, X., & Liang, S. (2015). Adomian decomposition method is a special case of Lyapunov's artificial small parameter method. *Applied Mathematics Letters*, 48, 177-179.
- [10] Liao, S.J. (2003). *Beyond Perturbation: Introduction to the Homotopy Analysis Method*. Boca Raton: Chapman and Hall / CRC Press.

- [11] Liao, S.J. (2009). Notes on the homotopy analysis method: some definitions and theorems. *Communications in Nonlinear Science and Numerical Simulation*, 14, 983-997.
- [12] Liao, S.J. (2010). An optimal homotopy-analysis approach for strongly nonlinear differential equations. *Communications in Nonlinear Science and Numerical Simulation*, 15, 2003-2016.
- [13] Liao, S.J. (2014). *Advances in the Homotopy Analysis Method*. World Scientific Publishing.
- [14] Yadav, S., Keshav, S., Singh, S., Singh, M., & Kumar, J. (2023). Homotopy analysis method and its convergence analysis for a nonlinear simultaneous aggregation-fragmentation model. *Chaos, Solitons and Fractals*, 177, 14204.
- [15] Zaheer, M., Abbas, S.Z., Huang, N., & Elmasry, Y. (2024). Analysis of buoyancy features on magneto hydrodynamic stagnation point flow of nanofluid using homotopy analysis method. *International Journal of Heat and Mass Transfer*, 221, 125045.