

Canonical dynamics of the Nosé oscillator: Stability, order, and chaos

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Nosé has developed many-body equations of motion designed to reproduce Gibbs's canonical phase-space distribution. These equations of motion have a Hamiltonian basis and are accordingly time-reversible and deterministic. They include thermodynamic temperature control through a single deterministic friction coefficient, which can be thought of as a control variable or as a memory function. We apply Nosé's idea to a single classical one-dimensional harmonic oscillator. This relatively simple system exhibits both regular and chaotic dynamical trajectories, depending on the initial conditions. We explore both the nature of these solutions by examining their fractal dimensionality and Lyapunov instability. The Nosé oscillator in a frictionless case, not sufficiently chaotic for a fully statistical description. We suggest that the behavior of only slightly more complicated systems is considerably simpler and is accord with statistical mechanics.

I. INTRODUCTION AND MOTIVATION

During the past ten years an intensive effort has been made to use computers in the simulation of many-body systems in nonequilibrium states.¹ A major difficulty in achieving this goal had been the lack of useful controls over the thermodynamic independent variables. It is necessary to control temperature or pressure or energy in order to simulate nonequilibrium steady states far from equilibrium. The techniques of control theory can be applied to this problem, adding arbitrary "control forces" or "constraint forces" designed to maintain thermodynamic variables fixed. Some of these same constraint forces are suggested by classical mechanics. Gauss, for instance, made the reasonable suggestion that constraint forces should be made as small as is possible, in a least-square sense. The resulting principle of least constraint² is the most general formulation of classical mechanics. This principle leads to frictional forces, lower in the momentum, of the same form familiar from control theory.³ Much more recently, Nosé has suggested a frictional force designed to reproduce the statistical constant thermodynamic temperature and isotropic constant thermodynamic pressure phase-space distributions in equilibrium systems.^{4,5} Nosé's equations of motion incorporate "integral control" in which the friction coefficient, or "control variable," depends linearly on the integrated history of the system's kinetic energy.

Unlike hydrodynamic frictional forces, Gauss's and Nosé's forces are time-reversible. In fact, even far from equilibrium, the new equations, like Newton's, are purely deterministic and reversible.

Canonical ensemble equilibrium properties are not at all mysterious or hard to compute. There already exist many practical schemes for determining the thermodynamic and structural properties of many-body systems with great accuracy.⁶ Thus the new schemes have little to offer in the way of improving equilibrium simulations. Instead, Gauss's and Nosé's ideas are particularly promising because they suggest approaches to classes of problems in

nonequilibrium and quantum-mechanical simulation for which no useful theories exist. They also suggest ways of simplifying and analyzing deterministic and stochastic dynamics through the use of deterministic driving forces.

These ideas have already proved their usefulness in the study of nonequilibrium systems. The new equations make it possible to simulate, and to analyze theoretically, systems connected to thermal or mechanical reservoirs without the need for stochastic or irreversible forces. It is remarkable that this has been achieved with time-reversible equations. Thus a movie of a physically irreversible process described with a Gaussian or Nosé thermostat reproduces accurately the mathematical formal solution of the equations of motion only in the forward direction. Because the backward direction corresponds to an energy decrease, it cannot be observed in any finite-precision computation and the reversed movie represents a fictional trajectory.

Gauss's and Nosé's equations of motion have been applied to the study of fluid and solid diffusion,^{7,8} viscosity,^{9,10} and heat conduction^{11,12} with computer simulation and to the nonlinear generalization of linear response theory^{13,14} required to describe systems far from equilibrium.

In order to characterize these new dynamical approaches and to assist the development of the theory, it is essential to study their application to the simplest possible prototypical systems. In this way the advantages of the new methods can be exploited and the disadvantages recognized. Thus two-body^{15,16} and three-body¹⁷ nonequilibrium systems have been simulated using Gaussian and Nosé dynamics.

To help assess these new developments in nonequilibrium molecular dynamics we study here the one-dimensional harmonic oscillator using Nosé's controlled equations of motion.¹⁸ This is a problem with three time-dependent variables, the coordinate q , the momentum p , and the friction coefficient ζ . Each of these obeys a first-order differential equation of motion. The oscillator exhibits many of the familiar features found earlier in

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Table of Contents Ambulance Service Basic Training Manual A5

1. Understanding the eBook Ambulance Service Basic Training Manual A5
 - The Rise of Digital Reading Ambulance Service Basic Training Manual A5
 - Advantages of eBooks Over Traditional Books
2. Identifying Ambulance Service Basic Training Manual A5
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Ambulance Service Basic Training Manual A5
 - User-Friendly Interface
4. Exploring eBook Recommendations from Ambulance Service Basic Training Manual A5
 - Personalized Recommendations
 - Ambulance Service Basic Training Manual A5 User Reviews and Ratings

- Ambulance Service Basic Training Manual A5 and Bestseller Lists
- 5. Accessing Ambulance Service Basic Training Manual A5 Free and Paid eBooks
 - Ambulance Service Basic Training Manual A5 Public Domain eBooks
 - Ambulance Service Basic Training Manual A5 eBook Subscription Services
 - Ambulance Service Basic Training Manual A5 Budget-Friendly Options
- 6. Navigating Ambulance Service Basic Training Manual A5 eBook Formats
 - ePub, PDF, MOBI, and More
 - Ambulance Service Basic Training Manual A5 Compatibility with Devices
 - Ambulance Service Basic Training Manual A5 Enhanced eBook Features
- 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Ambulance Service Basic Training Manual A5
 - Highlighting and Note-Taking Ambulance Service Basic Training Manual A5
 - Interactive Elements Ambulance Service Basic Training Manual A5
- 8. Staying Engaged with Ambulance Service Basic Training Manual A5
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Ambulance Service Basic Training Manual A5
- 9. Balancing eBooks and Physical Books Ambulance Service Basic Training Manual A5
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Ambulance Service Basic Training Manual A5
- 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
- 11. Cultivating a Reading Routine Ambulance Service Basic Training Manual A5
 - Setting Reading Goals Ambulance Service Basic Training Manual A5
 - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Ambulance Service Basic Training Manual A5
 - Fact-Checking eBook Content of Ambulance Service Basic Training Manual A5
 - Distinguishing Credible Sources

13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
14. Embracing eBook Trends
 - Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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