



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 how 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.

1. 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 technique 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-squares sense. The resulting principle of least constraint² is the most general formulation of classical mechanics. This principle leads to frictional forces, known in the literature, of the same form familiar from control theory.³ Much more recently, Nosé has suggested a frictional force designed to reproduce the canonical constant thermodynamic temperature and isochoric (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 unifying 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 represents accurately the mathematical formal solution of the equations of motion only in the forward direction. Because the backward direction corresponds to an entropy 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 simulations 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 canonical 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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