# Thermostat algorithm for generating target ensembles

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We present a deterministic algorithm called contact density dynamics that generates any prescribed target distribution in the physical phase space. Akin to the famous model of Nosé and Hoover, our algorithm is based on a non-Hamiltonian system in an extended phase space. However, the equations of motion in our case follow from contact geometry and we show that in general they have a similar form to those of the so-called density dynamics algorithm. As a prototypical example, we apply our algorithm to produce a Gibbs canonical distribution for a one-dimensional harmonic oscillator.

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## I. INTRODUCTION

Equilibrium statistical mechanics is a beautiful mathematical construction based on Gibbs canonical distribution and a very powerful tool that permits to establish a link between the microscopic laws of motion and the macroscopically observable properties of systems with a large number of particles. However, some conceptual and practical problems in this framework are still unsettled.

A major issue regards the mechanical foundations of the equilibrium distribution. In fact, the dynamical evolution of a Hamiltonian system is confined to a hypersurface of constant energy of the phase space and therefore the only possible distribution for the energy of the system from a dynamical perspective is a $\delta$ distribution, which represents the microcanonical ensemble. Therefore, a relevant problem at the foundations of statistical mechanics, which is also of primary practical importance for numerical simulations, is that of finding a well-defined dynamics that can lead to ensembles which are different from the microcanonical one. In this case several proposals have been found, which are generally based on defining a fictitious dynamical system in an extended phase space that reduces to the desired non-Hamiltonian dynamics in the physical phase space, with the property that the invariant distribution reproduces a specified ensemble. Such algorithms are known in the literature as *thermostat algorithms*. The paradigmatic example is the Nosé-Hoover (NH) algorithm, which generates the canonical ensemble in the physical phase space [1] (see also [2–8] for further references).

In [9] an algorithm based on the NH idea that generates *any* distribution on the physical phase space was proposed, which is called *density dynamics* (DD). Here we introduce an algorithm similar in spirit to that of DD. The main difference is that our procedure is motivated through a geometrical setting. In fact the systems that we introduce are the natural extension of classical Hamiltonian systems to a space with an extra dimension and are known in the literature as *contact Hamiltonian systems* [10,11]. Their dynamics includes standard Hamiltonian dynamics in some particular cases that we point out. However, in the general case it is more rich and we show that this generality is the essential ingredient to allow for the dynamical generation of ensembles different from the microcanonical one. For this reason we refer to our algorithm as *contact density dynamics* (CDD).

To introduce our algorithm we proceed in three steps, akin to the NH and DD procedures. We start with a class of dynamical systems in an extended phase space, which in our case is given by contact Hamiltonian systems. The second step is to find an invariant measure for their flow. This step was pursued in [12], where the important fact was remarked that there is a *unique* invariant measure depending only on the generating function in the extended phase space. Finally, the last step is to show that, by a proper choice of the generating function and by integrating out the additional unphysical degree of freedom, any desired distribution in the physical phase space can be generated. We argue that, assuming that the dynamics in the extended phase space is ergodic, our results provide a dynamical foundation for different ensembles. To show that this is indeed the case, we include a numerical simulation generating a Gibbs canonical ensemble for a one-dimensional harmonic oscillator.

In what follows we first introduce the basics of NH and DD algorithms and then present our proposal. To fix the notation, we always denote by $\Gamma$ the physical phase space, with variables $(p,q)$, where $p$ and $q$ are $n$-dimensional vectors and $n$ is the number of degrees of freedom of the system. Moreover, $\tilde{\Gamma}$ indicates the extended phase space, a $(2n+1)$-dimensional space with coordinates $(p,q,S)$.

## II. NOSÉ-HOOVER ALGORITHM AND DENSITY DYNAMICS

### A. Nosé-Hoover algorithm

The logic of the NH algorithm follows three steps. Step 1 is simply the definition of a dynamical system in $\tilde{\Gamma}$, given by

$$\dot{q}_i = \frac{\partial H(p,q)}{\partial p_i}, \tag{1}$$

$$\dot{p}_i = -\frac{\partial H(p,q)}{\partial p_i} - S\, p_i, \tag{2}$$

$$\dot{S} = \frac{1}{Q}\left(\sum_{i=1}^{n} p_i \frac{\partial H(p,q)}{\partial p_i} - \frac{n}{\beta}\right), \tag{3}$$

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where $p_i$ and $q_i$ are the physical positions and momenta, and $Q$ is a positive constant and $\beta = 1/k_B T$. Here $S$ is an additional variable introduced *ad hoc* in order to generate a non-Hamiltonian dynamics on $\Gamma$ with the desired property of having control over the temperature $T$. Furthermore, $H(p,q)$ is the Hamiltonian of the system. Step 2 is the identification of an invariant measure on $\tilde{\Gamma}$. It turns out (see, e.g., [3]) that the system (1)–(3) has the invariant measure

$$\mathrm{d}\mu_{\mathrm{NH}} = e^{-\beta H(p,q)}\, e^{-\beta Q S^2/2}\, d^n p\, d^n q\, dS, \tag{4}$$

where $d^n p\, d^n q\, dS$ is the volume element of $\tilde{\Gamma}$.

Step 3 consists of obtaining the corresponding measure on $\Gamma$ by integrating out the additional variable $S$. A direct integration in Eq. (4) gives (up to a multiplicative factor)

$$d\mu_{\mathrm{NH}}|_{\Gamma} = e^{-\beta H(p,q)} d^n p\, d^n q, \tag{5}$$

which coincides with the canonical measure. This proves that NH dynamics can generate the canonical ensemble in the physical phase space, provided the dynamics (1)–(3) is ergodic [2,13].

### B. Density dynamics

The DD algorithm aims to generalize the NH equations in order to yield any distribution on the physical phase space. The key idea of DD is to define an *ad hoc* dynamical system on $\tilde{\Gamma}$ with the property that its invariant distribution coincides with an arbitrary $\rho(p,q,S)$. Then $\rho(p,q,S)$ is projected to $\Gamma$ to obtain the desired distribution. To do so, one starts with the function

$$\Theta(p,q,S) = -\ln \rho(p,q,S) \tag{6}$$

and writes the flow

$$\dot{q}_i = \frac{\partial \Theta(p,q,S)}{\partial p_i}, \tag{7}$$

$$\dot{p}_i = -\frac{\partial \Theta(p,q,S)}{\partial q_i} - \frac{\partial \Theta(p,q,S)}{\partial S}\, p_i, \tag{8}$$

$$\dot{S} = \sum_{i=1}^{n} p_i \frac{\partial \Theta(p,q,S)}{\partial p_i} - n. \tag{9}$$

It can be checked then that Liouville equation $\mathrm{div}\rho X = 0$ is satisfied, with $X$ the vector field generating the flow (7)–(9). Therefore, $\rho(p,q,S)$ is the invariant distribution on $\tilde{\Gamma}$. For instance, when $\Theta(p,q,S) = \beta[H(p,q) + QS^2/2]$ one recovers the NH case with the distribution (4).

A simple and very useful case is the one in which the invariant distribution $\rho(p,q,S)$ is of the form

$$\rho(p,q,S) = \rho_{\mathrm{t}}(p,q)\, f(S), \tag{10}$$

where $\rho_{\mathrm{t}}(p,q)$ is the target distribution on $\Gamma$ and $f(S)$ is a normalized distribution for the thermostatting variable $S$. Equation (10) being a product of two independent distributions, the integration of the variable $S$ is straightforward and the result is the desired distribution $\rho_{\mathrm{t}}(p,q)$ in the physical phase space.

In the following we present our algorithm for generating equilibrium ensembles. As for the above description of the NH algorithm, we divide it into three steps and we show that, although it is derived from a geometric perspective, it retains all the positive features of the DD algorithm.

## III. CONTACT DENSITY DYNAMICS

### A. Step 1: Contact Hamiltonian systems

Contact Hamiltonian systems are defined in a precise geometric fashion starting from a generating function in the extended phase space which we indicate as $h(p,q,S)$. The function $h$ is called the *contact Hamiltonian* of the system (for more details see, e.g., [10–12]). The properties of such systems have already been exploited in physics. In particular, they are relevant in thermodynamics [14–18] and in control theory [19,20]. Recently, it was also proposed that they can be suitable to study the statistical mechanics of nonconservative systems [12] and to improve the efficiency of Monte Carlo simulations [21]. For our discussion, it is sufficient to write down the dynamical equations thus generated, which read

$$\dot{q}_i = \frac{\partial h(p,q,S)}{\partial p_i}, \tag{11}$$

$$\dot{p}_i = -\frac{\partial h(p,q,S)}{\partial q_i} + \frac{\partial h(p,q,S)}{\partial S}\, p_i, \tag{12}$$

$$\dot{S} = -\sum_{i=1}^{n} p_i \frac{\partial h(p,q,S)}{\partial p_i} + h(p,q,S). \tag{13}$$

From Eqs. (11) and (12) it is clear that this dynamics induces a standard Hamiltonian dynamics over the physical phase space whenever the generating function $h$ does not depend on $S$. In addition, the similarity with the NH and DD equations is evident and is made more concrete in the next section; cf. Eqs. (17)–(19).

### B. Step 2: The invariant distribution for contact Hamiltonian systems

Although the system (11)–(13) is non-Hamiltonian and there is no conserved quantity in the general case, it was found in [12] that there is only one invariant measure on $\tilde{\Gamma}$ which depends uniquely on $h$ whenever $h \neq 0$. This is given by

$$d\mu = \frac{|h|^{-(n+1)}}{\mathcal{Z}_n}\, d^n p\, d^n q\, dS, \tag{14}$$

where $|\cdot|$ is the absolute value and $\mathcal{Z}_n$ is the partition function. Thus, Eq. (14) shows that the invariant measure of the dynamics generated by any contact Hamiltonian system in the extended phase space has a power law distribution. We show below that, for a proper choice of $h$, the invariant measure (14) induces any desired distribution on $\Gamma$, just as in the DD case.

### C. Step 3: Integrating out $S$ and recovering the target distribution

Let us proceed as in the preceding discussion about DD and assume that we wish to induce the *target* distribution $\rho_{\mathrm{t}}(p,q)$ on $\Gamma$. Considering the measure (14), together with the choice of the contact Hamiltonian

$$h(p,q,S) = [\rho_{\mathrm{t}}(p,q) f(S)]^{-\frac{1}{n+1}}, \tag{15}$$

it turns out that the invariant distribution on $\tilde{\Gamma}$ is set to be Eq. (10). Moreover, with the choice of $h$ as in Eq. (15), the function $h$ is always positive and therefore the absolute value in Eq. (14) is not necessary and we avoid regions where $h = 0$ and the invariant measure is degenerate.

Now, since $f(S)$ is a normalized distribution by assumption, we can integrate out the unphysical degree of freedom, $S$, and obtain the induced measure on $\Gamma$, which is

$$d\mu|_\Gamma = \rho_t(p,q)\, d^n p\, d^n q. \tag{16}$$

This concludes our algorithm for generating any desired ensemble on the physical phase space.

Notice that different choices of the target distribution lead to different $h$ in Eq. (15) and therefore to different dynamical equations of the form (11)–(13). Moreover, Eq. (15) is not the only possibility for the generating function. We decided to present this form for clarity because in this case it is particularly simple to integrate out $S$. A comment on ergodicity is also in order. Since $h$ as in Eq. (15) is always greater than zero, the flow equations (11)–(13) do not have any fixed points, which are obstructions to ergodicity. Finally, from the form of $h$ as in Eq. (15), the dynamical equations on $\tilde{\Gamma}$ take the form

$$\dot{q}_i = \frac{h}{n+1}\frac{\partial\Theta(p,q,S)}{\partial p_i}, \tag{17}$$

$$\dot{p}_i = \frac{h}{n+1}\left[-\frac{\partial\Theta(p,q,S)}{\partial q_i} + \frac{\partial\Theta(p,q,S)}{\partial S}\, p_i\right], \tag{18}$$

$$\dot{S} = \frac{h}{n+1}\left[-\sum_{i=1}^{n} p_i \frac{\partial\Theta(p,q,S)}{\partial p_i} + n + 1\right], \tag{19}$$

where $\Theta$ is given by Eq. (6). These equations suggest that the CDD algorithm is a rescaling of the DD algorithm on the extended phase space by the positive function $h/(n+1)$. The relationship between CDD and DD is beyond of the scope of this work and it will be explored in future efforts. Having established our algorithm, in the next section we apply it to a concrete example, the generation of Gibbs canonical distributions for a one-dimensional harmonic oscillator.

## IV. NUMERICAL SIMULATION

In this section we consider a one-dimensional harmonic oscillator and show that our algorithm produces a Gibbs canonical distribution in the physical phase space. This is a standard test for thermostat algorithms [2–5,22]. For instance, it has been shown that the NH equations cannot generate a Gibbs ensemble for this system due to the lack of ergodicity [1,2,23,24].

Following Eq. (15), the contact Hamiltonian for this system is

$$h(p,q,S) = \left(\frac{e^{-\beta H(p,q)}}{\mathcal{Z}} f(S)\right)^{-1/2}, \tag{20}$$

with $H(p,q)$ the Hamiltonian function of a harmonic oscillator with potential $U(q) = 2q^2$, $\mathcal{Z} = \pi/\beta$ the corresponding partition function, and $f(S)$ a normalized distribution. The freedom in $f(S)$ allows us to do numerical tests for different distributions and choose the most adequate according to the ergodicity of the corresponding dynamical system and to the computational cost of the numerical integration of the equations of motion. Considering these issues, we select $f(S)$

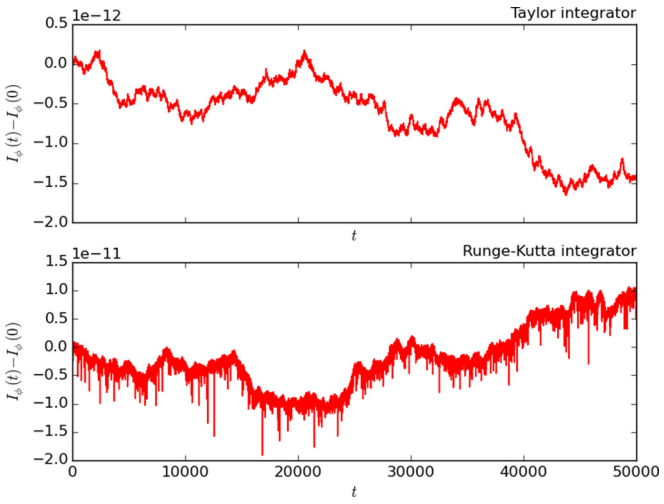


FIG. 1. Evolution of the error in the invariant quantity (22) for both the RK and the TS integrators with same random initial condition.

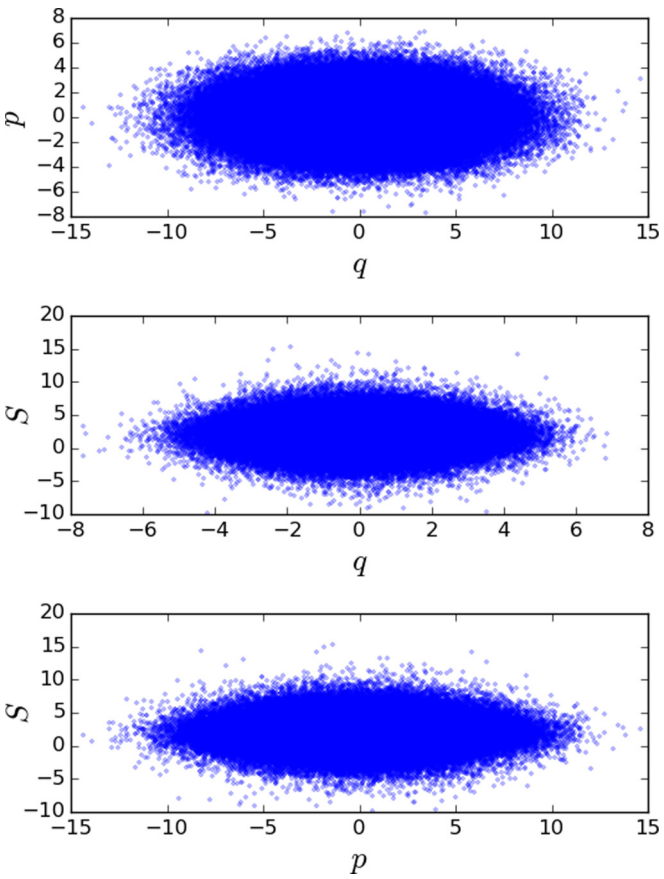


FIG. 2. Projections of the extended phase space orbit of a one-dimensional harmonic oscillator in the $(p,q)$, $(S,q)$, and $(S,p)$ planes. An orbit with $3 \times 10^5$ points is shown. Initial condition $[q_0,p_0,S_0] = [0.12578471404894542, 0.7479637648489665, 0.917435858684718]$. More details are available in the text.

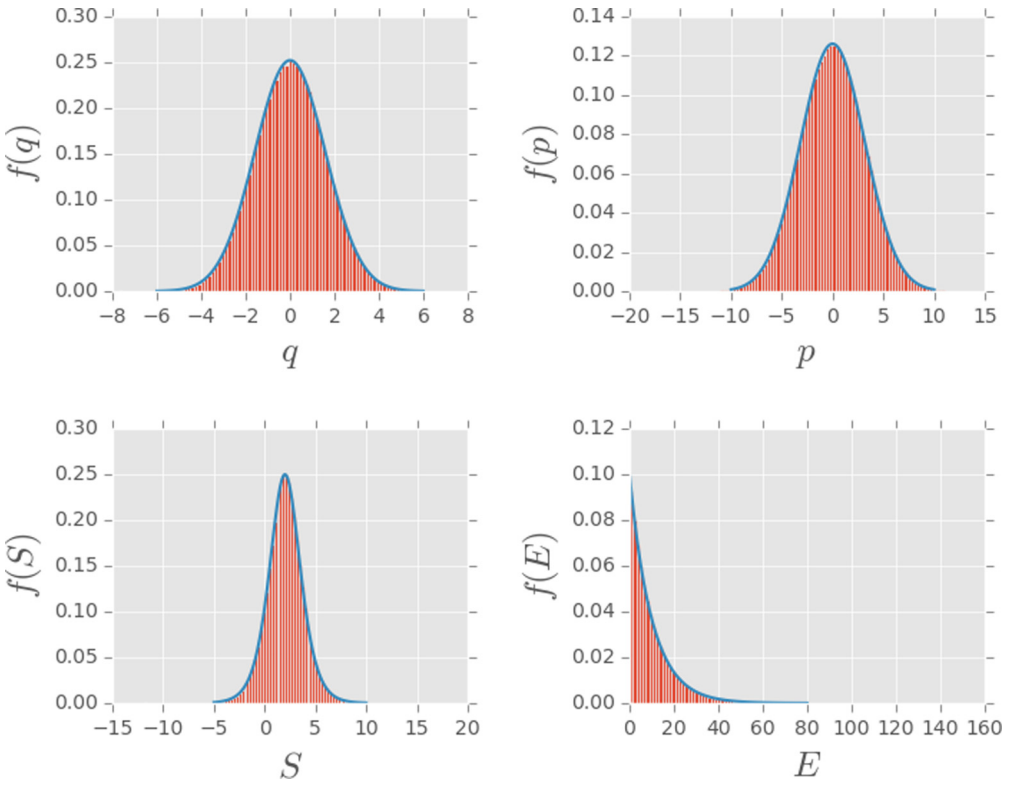


FIG. 3. Histograms of the frequencies for $q$, $p$, $S$, and $E$ and corresponding theoretical distributions (solid line) for a one-dimensional harmonic oscillator. The initial condition is the same as for Fig. 2. More details are available in the text.

to be the logistic distribution with scale 1 and mean $c$; that is,

$$f(S;c) = \frac{e^{S-c}}{(1+e^{S-c})^2}. \tag{21}$$

The choice of the numerical value of $c$ is also guided by the same principles mentioned above (ergodicity and computational cost). For the simulation we fix $c = 2$, $k_B = m = 1$, and $\beta = 0.1$. It has been also argued that having the additional freedom in the choice of unknown functions such as our $f(S)$, which affects the dynamics but not the equilibrium properties, may help to extend the capability to adequately simulate not only static averaged but also transport and time-dependent properties (see, e.g., [25]). A detailed analysis of such nonequilibrium properties is beyond the scope of the present work and will be addressed elsewhere.

To integrate the equations of motion we use and compare two different integration schemes, the standard Runge-Kutta (RK) and the Taylor series (TS) method for ordinary differential equations [26–28]. We have implemented both of them by means of a JULIA code and made them available at [29]. The RK scheme adopted is the fourth order adaptive with Dormand-Prince coefficients [30], with a relative tolerance of $1.0 \times 10^{-16}$ and an absolute tolerance of $1.0 \times 10^{-20}$. On the other hand, the order taken in the TS method is 28 with a variable step size and a tolerance of $1.0 \times 10^{-20}$. Since the step size in the methods is not constant, we need to fix a sample time. We choose $\Delta t_{\text{sample}} = 0.05$ and we decide to stop the simulation after a number of samplings $n_{\text{sampling}} = 1 \times 10^6$, which corresponds to a total integration time $t_{\text{total}} = \Delta t_{\text{sample}} \times n_{\text{sampling}} = 5 \times 10^4$.

In order to check the accuracy of the two methods for the integration of the equations of motion, we have resorted to a test proposed in [31]. In this work the authors derive an invariant quantity for an arbitrary system of differential equations

$$I_\phi(t) = -\ln \rho(\phi(t)) + \int_0^t \text{div} X(\phi(s))ds, \tag{22}$$

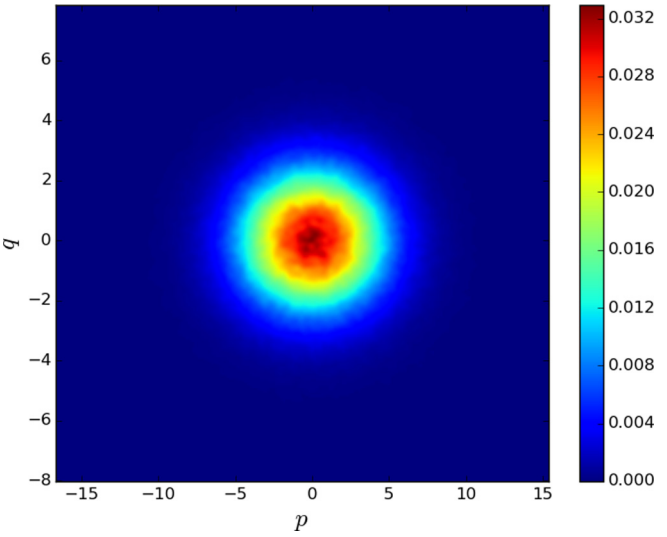


FIG. 4. Numerical joint probability distribution for $p$ and $q$ for a one-dimensional harmonic oscillator. The initial condition is the same as for Fig. 2. More details are available in the text.

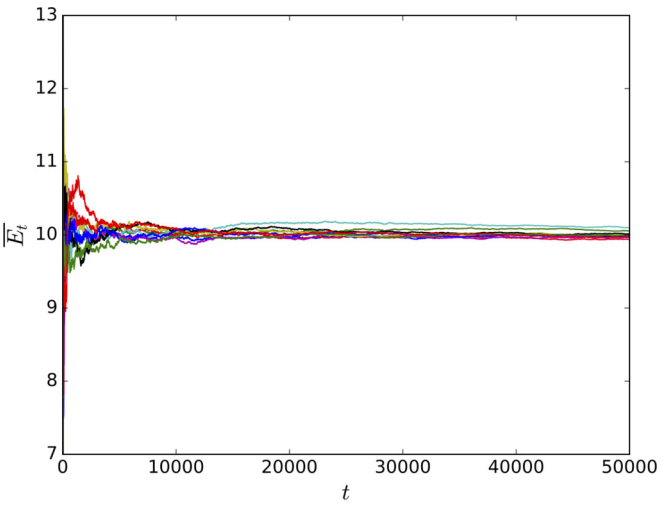


FIG. 5. Time average of the energy as a function of time for ten different initial conditions. Details are available in the text.

where $\rho$ is the invariant distribution of the dynamics, $\phi$ is the flow that gives the time evolution, $X$ is the vector field generating the dynamics, and div stands for the divergence. Since $I_\phi$ is an invariant quantity, its value at any time $t$ must be the same as the initial value. Therefore, this provides a useful test for the accuracy of the numerical integration. For the time of integration considered, the RK method numerically conserves the invariant (22) with an error of less than few parts in $1 \times 10^{11}$, while the TS integrator conserves (22) with an error of less than few parts in $1 \times 10^{12}$ (see Fig. 1). This is a good indication of the validity of both methods to integrate the equations of motion. All the tests with the two different schemes can be checked in [29]. In what follows we show only the results of the integration performed with the Taylor series method.

In Fig. 2 we display the projections to different planes of the orbit of the system with a randomly generated initial condition. We see that the phase space is filled by the orbit. We have analyzed the orbits of $1 \times 10^3$ different random initial conditions and checked that the filling of the phase space is a generic property, which suggests the ergodicity of the system.

In Fig. 3 we show the histograms of the frequencies of the numerical values of $q, p, S$ and $E = H(p,q)$ for the specified trajectory and compare them with their theoretical distributions. The histograms are in good agreement with the theoretical curves. Figure 4 displays the numerical joint probability distribution of $p$ and $q$ along the orbit. The Gaussian character of the bivariate distribution is clearly observed. All these tests indicate that the CDD correctly generates Gibbs distributions for this system.

As a final examination, we compute the time averages of the energy $\overline{E_t}$ for an *ensemble* of $1 \times 10^2$ oscillators and compare them with the ensemble average $\langle E \rangle = 1/\beta = 10.0$. At the final time $t_{\text{total}}$ the relative error for each element of the ensemble is less than 2%. In Fig. 5 we plot the evolution of $\overline{E_t}$ for ten representative elements. The convergence of the time averages to the ensemble average of the energy is a further indication of the ergodicity of the system.

## V. CONCLUSIONS

Hamiltonian mechanics and symplectic geometry are at the foundations of equilibrium statistical mechanics of conservative systems since they produce the microcanonical ensemble. Here we have proposed an algorithm based on contact geometry and the corresponding Hamiltonian systems that dynamically produces any desired ensemble. This might provide a theoretical basis for the equilibrium statistical mechanics of nonconservative systems.

We have shown that our algorithm generates equations of motion which have the same structure of those provided by density dynamics. However, the main difference between our algorithm and DD is that our framework is grounded on the geometry of the extended phase space.

To investigate the ergodicity of the dynamics induced by our algorithm and prove that it effectively yields the desired target distribution in the physical phase space, we have presented an example in which we simulated a one-dimensional harmonic oscillator in a Gibbs canonical ensemble. We have considered different curves in the phase space, marginal and joint distributions, and the time averages of the energy for several randomly generated initial conditions. From all these tests we conclude that the system is in the canonical ensemble, as expected.

In future works we wish to clarify in detail the relationship between our algorithm and density dynamics and to study the physical relevance of the contact Hamiltonian. Moreover, we are going to apply the present proposal to construct several systems in different ensembles. We consider that our contact density dynamics algorithm can be useful in the design of molecular dynamics simulations and that it establishes a step forward in the theoretical understanding of equilibrium in nonconservative systems.

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