

# On the Geometry of Non-Hamiltonian Phase Space

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In this paper the statistical mechanics of canonical, non-canonical and non-Hamiltonian systems is analyzed rigorously by throwing light onto the peculiar geometric structure of phase space. Misleading points, regarding generalized brackets and Jacobi relations, are clarified. The accessory role of phase space compressibility in the statistical mechanics of non-canonical and non-Hamiltonian systems is also unveiled. A rigorous definition of the (relative) entropy for continuous probability distributions is adopted and used in order to introduce maximum entropy principles for non-canonical and non-Hamiltonian systems. Although the attention is concentrated on the geometry of phase space under equilibrium thermodynamic conditions, the results and the points of view presented lay the foundations for a maximum entropy approach to non-Hamiltonian dissipative systems.

## I. INTRODUCTION

In the field of classical mechanics, non-Hamiltonian formalisms were developed in order to simulate numerically the effect of thermal and pressure bath on relevant subsystems by means of a finite number of degrees of freedom<sup>1-4</sup>. In quantum mechanics, non-Hamiltonian theories are able to describe consistently the coupling of quantum and classical degrees of freedom<sup>5,6</sup>. Classical non-Hamiltonian theories in phase space are presently formulated by means of two different approaches. In the first of these, phase space is considered as a Riemann manifold, endowed with a metric tensor whose determinant is used to define the measure of the volume element<sup>7-9</sup>. Within this approach is not clear how to derive non-Hamiltonian equations of motion but, once these are given in some way, their statistical mechanics is defined *via* the introduction of an invariant measure of phase space. The other approach, originated mainly by this author, uses generalized antisymmetric brackets to define non-Hamiltonian equations of motion<sup>10,11</sup>. By means of these brackets a generalized Liouville equation for distribution functions in phase space can be written down. Solutions of the Liouville equation give the statistical weight of phase space. In this formalism, the concept of invariant measure can also be introduced. This approach has an algebraic (group theoretical structure) whose distinctive feature is the violation of the Jacobi relation<sup>12,13</sup>. Therefore, linear response<sup>10,11</sup> theory and extensions to quantum and quantum-classical mechanics<sup>6</sup> are easily formulated.

Recently, a paper by Tarasov<sup>9</sup> has tried to find a link between these two different mathematical languages by claiming to introduce non-Hamiltonian brackets which satisfy the Jacobi relation. The work of Tarasov is interesting and valuable in many aspects but, unfortunately, risks to generate confusion in the literature because of the use of the Riemann formalism and of a different, and not entirely correct, definition of non-Hamiltonian systems. As a matter of fact, a non-Hamiltonian bracket satisfying the Jacobi relation is an oxymoron: if a bracket satisfies the Jacobi relation then, because of a theorem

due to Darboux<sup>14</sup>, the dynamics can be transformed, at least locally, in Hamiltonian form, as thoroughly discussed in Ref.<sup>15</sup>. One can indeed write the equality “Jacobi relation satisfied = Hamiltonian phase space” (with phase space expressed either in canonical or non-canonical coordinates). In non-canonical Hamiltonian phase space, the brackets (which arise from a generalization of the symplectic structure of the canonical case) always satisfy the Jacobi relation: such brackets are called non-canonical<sup>13,15</sup>. As shown by this author<sup>6,10,11</sup>, generalizing further antisymmetric brackets one violates the Jacobi relation and obtains certain types of non-Hamiltonian dynamics. One could write the equation “Failure of the Jacobi relation = non-Hamiltonian dynamics”. When generalized brackets can be used in order to define non-Hamiltonian phase space flows the Jacobi relation cannot be satisfied. Phase space compressibility may or may not be present. It is not yet clear if more general types of non-Hamiltonian dynamics, for example dissipative flows, may be described by generalized brackets. In this more general cases, one can always resort to Liouville operators.

One subtle issue, which arises when using ‘metric’ formalisms<sup>7-9</sup> in non-Hamiltonian statistical mechanics, is the fact that phase space, either in the canonical, non-canonical or non-Hamiltonian case, is not a *natural* Riemann manifold: there is no metric tensor and no length associated to the line element. This is trivial in the canonical Hamiltonian case<sup>12,13</sup>: generalized coordinates (angles, areas and so on) are defined on Cartesian axis and translations along the axes always commute. In non-canonical coordinates, and with a non-zero compressibility, there is also no *natural* metric tensor because one cannot define a physically meaningful length of the line element. Jacobi relation is still satisfied, which means that by Darboux’s theorem<sup>14,15</sup> one can always regain the canonical Hamiltonian form, but translations along the axes do no longer commute: in non-canonical coordinates phase space is a curved manifold with a non-trivial affine connection<sup>16-18</sup>. Nevertheless, it should be known that there is no need to define a metric to introduce non-trivial parallel transport into a manifold: non-trivial affine connections can be introduced with-

out referring to metric properties<sup>16,17</sup>. Thus, in non-canonical Hamiltonian phase spaces one can have a curvature and a non-trivial parallel transport but still no need to introduce a metric tensor. Once one accepts the fact that a space can be affinely connected without a metric tensor<sup>16,17</sup>, analogous considerations can be applied to the non-Hamiltonian case. Thus, rigorously speaking, phase space is not a Riemann space endowed with a metric. Precisely because there is no *natural* metric, one can choose any metric tensor to express, for example, distances between trajectories starting from close initial conditions (as it is done in studies of chaotic dynamics). However, in non-canonical coordinates there is a non-trivial measure, given by the Jacobian of the transformation from canonical to non-canonical coordinates, which must be used to define the volume element needed in order to define statistical mechanics. In the non-Hamiltonian case, things are more subtle but similar considerations can be done. As a matter of fact, in ‘metric’ theories<sup>7–9</sup> of statistical mechanics, the metric tensor is introduced fictitiously and uniquely to define the volume element of phase space.

It can be guessed from the previous discussion that systems with a non-zero phase space compressibility are not necessarily non-Hamiltonian. For example, non-canonical systems are Hamiltonian but may have a non-zero compressibility<sup>15</sup>. Non-Hamiltonian systems, i.e. systems which violate the Jacobi relation, may also have a zero compressibility. Examples will be given in the following sections. Therefore, it must be understood that the mere existence of the compressibility does not imply at all that the dynamics, the brackets, and the phase space are non-Hamiltonian. For non-canonical phase space, this is very clearly discussed in Ref.<sup>15</sup> by means of non-canonical brackets that satisfy the Jacobi relation. Non-canonical and non-Hamiltonian systems with a zero compressibility are particularly subtle because, in such cases, ‘metric’ recipes<sup>7–9</sup> for defining the invariant measure, and for separating the statistical,  $f(x)$ , from the geometric contributions,  $m(x)$ , in the distribution function,  $\rho(x) = m(x)f(x)$ , simply do not work (with  $x$  one denotes phase space coordinates, collectively). Instead, solutions of the generalized Liouville equation always give the statistical distribution function to be used in the calculations of averages and linear response theory<sup>10,11</sup>. Moreover, from the presentation given in some papers<sup>7</sup>, it seems that the knowledge of  $\rho(x)$  alone would lead to an incorrect definition of the entropy functional. This too must be clarified. In practice, the entropy functional, as already discussed in Refs.<sup>19–21</sup>, can be defined without any knowledge of the ‘metric’ factor. The fundamental point to grasp is that for continuous probability distributions one must use the so-called relative entropy because the *absolute* entropy is ill defined<sup>21</sup>. The relative entropy functional naturally takes into account unknown ‘metric’ factors which, therefore, become superfluous. In conclusion, it turns out that the knowledge of  $\rho(x)$  is enough for a correct formalization of statistical mechan-

ics in the canonical, non-canonical, and non-Hamiltonian case.

In order to clarify all the above issues within this paper, formalisms and entropy for canonical, non-canonical, and non-Hamiltonian systems are discussed with a particular sensibility toward the peculiar geometric structure of phase space. Therefore, a rigorous approach to the statistical mechanics of non-canonical<sup>15,20</sup> and non-Hamiltonian systems<sup>10,11</sup> is given. A maximum entropy principle is introduced for non-canonical and non-Hamiltonian systems. It is worth to remark that, although this paper addresses mainly the geometry of phase space under equilibrium thermodynamic conditions, the maximum entropy principle can be easily extended to non-equilibrium ensembles. As a matter of fact, a recent work on the formulation of non-equilibrium non-Hamiltonian statistical mechanics<sup>22</sup> could be put on a more rigorous ground by means of the maximum entropy formalism presented in this paper. Nevertheless, it must be noted that non-Hamiltonian dissipative systems impose a fractal nature to phase space<sup>23</sup>. However, the perspective suggested in this paper, which avoids the definition of fictitious metric tensors in phase space and stresses, by means of the maximum entropy principle, the information theoretic content of statistical mechanics, could prove useful in avoiding the problems related to such a peculiar structure of dissipative phase space. Due to the controversial and subtle nature of this problem, extensions of non-Hamiltonian statistical mechanics to dissipative systems will be addressed in future papers.

This paper is organized as follows. In Sec. II canonical Hamiltonian phase space is briefly reviewed. The peculiar geometry of canonical phase space and its statistical mechanics are shortly discussed. The rigorous relative entropy concept is used and a ‘maximum relative entropy’ principle is formulated. Section III extends the result of Sec. II to non-canonical Hamiltonian phase space flows. Section IV extends the results of Sec. III to non-Hamiltonian phase space flows. Conditions in order to obtain non-Hamiltonian phase space flows with zero compressibility are derived. Appendices A and B provide examples of simple non-canonical and non-Hamiltonian dynamics, respectively, with zero compressibility. Finally, conclusions are given in Sec. V.

## II. CANONICAL HAMILTONIAN PHASE SPACE

Let  $x = (q, p)$  denote the point of phase space, where  $q$  and  $p$  are generalized coordinates and momenta, respectively. Let  $\mathcal{H}(x)$  be the generalized energy function of the system, or Hamiltonian. For simplicity, here and in the following section, the case in which  $\mathcal{H}(x)$  is time-independent will be considered. If  $2n$  is the dimension of phase space, let the  $2n \times 2n$  antisymmetric matrix  $\mathcal{B}^s$ , or

cosymplectic form<sup>12-15</sup>, be

$$\mathcal{B}^s = \begin{bmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{bmatrix}. \quad (1)$$

Then, canonical Hamiltonian equations of motion are given by

$$\dot{x}_i = \sum_{j=1}^{2n} \mathcal{B}_{ij}^s \frac{\partial \mathcal{H}}{\partial x_j}, \quad (2)$$

for  $i = 1, \dots, 2n$ . Equations (2) can be derived from a variational principle in phase space<sup>24</sup> applied to the action written in symplectic form

$$\mathcal{A} = \int dt \left[ \sum_{i,j=1}^{2n} \frac{1}{2} \dot{x}_i \mathcal{B}_{ij}^s x_j - \mathcal{H} \right]. \quad (3)$$

The compressibility of phase space is zero

$$\kappa = \sum_{i=1}^{2n} \frac{\partial \dot{x}_i}{\partial x_i} = \sum_{i,j=1}^{2n} \frac{\partial \mathcal{B}_{ij}^s}{\partial x_i} \frac{\partial \mathcal{H}}{\partial x_j} = 0, \quad (4)$$

because the matrix  $\mathcal{B}^s$  is constant. Poisson brackets can be defined as

$$\{a(x), b(x)\}_P = \sum_{i,j=1}^{2n} \frac{\partial a}{\partial x_i} \mathcal{B}_{ij}^s \frac{\partial b}{\partial x_j}, \quad (5)$$

where  $a(x)$  and  $b(x)$  are arbitrary phase space functions, so that equations of motion can be re-written as

$$\dot{x}_i = \{x_i, \mathcal{H}\}_P. \quad (6)$$

The Jacobi relation

$$\{a, \{b, c\}_P\}_P + \{c, \{a, b\}_P\}_P + \{b, \{c, a\}_P\}_P = 0 \quad (7)$$

is satisfied as an identity in canonical coordinates. Coordinates  $x$  are called canonical because

$$\{x_i, x_j\}_P = \mathcal{B}_{ij}. \quad (8)$$

It is well-known that Poisson brackets can be used to realize infinitesimal contact transformations<sup>12-14</sup>. In particular

$$\hat{T}_q = \{\dots, p\}_P \delta q \quad (9)$$

is the operator realizing infinitesimal translations along the  $q$  axis and

$$\hat{T}_p = -\{\dots, q\}_P \delta p \quad (10)$$

is the operator realizing infinitesimal translations along the  $p$  axis (i.e. infinitesimal changes of the generalized momenta). As a matter of fact, it can be easily verified that  $\hat{T}_q a(x) = (\partial a / \partial q) \delta q$  and  $\hat{T}_p a(x) = (\partial a / \partial p) \delta p$ .

It is easy to verify that, because of the canonical relations in (8), translations along the axis of different generalized coordinates, positions and momenta, commute. This means that canonical phase space is flat even if generalized coordinates are used and even if the Lagrangian manifold from which one builds phase space is a Riemann manifold<sup>13</sup>.

It is well known that the Liouville operator can also be introduced by using Poisson brackets,  $i\hat{L} = \{\dots, \mathcal{H}\}_P$ , and that the Liouville equation for the statistical distribution function in phase space is written<sup>25</sup>

$$\frac{\partial \rho(x)}{\partial t} = -i\hat{L}\rho(x). \quad (11)$$

In Equation (11), the function  $\rho(x) = \mathcal{J}^{can} f(x)$  has been introduced, where  $f(x)$  is the true distribution function in phase space and  $\mathcal{J}^{can} = 1$  is the Jacobian of transformations between canonical coordinates. In the canonical case,  $\rho(x) = f(x)$  trivially, however this notation will turn out to be convenient in later sections. By means of the Liouville operator one can introduce the propagator  $\exp[it\hat{L}] = \exp[it\{\dots, \mathcal{H}\}_P]$  whose action is defined by

$$a(x(t)) = \exp[it\hat{L}]a(x), \quad (12)$$

where it is assumed that by writing  $x$  without the time argument its value at time zero must be understood. Statistical averages are calculated as

$$\langle a(x) \rangle = \int dx \rho(x) a(x), \quad (13)$$

and correlation functions as

$$\langle ab(t) \rangle = \int dx \rho(x) a(x) \exp[it\hat{L}]b(x). \quad (14)$$

All the above is very well known and it is indeed a textbook subject<sup>13,25</sup>. Although there are some important exceptions<sup>20</sup>, what seems it is not shared by the community of researchers in the field of molecular dynamics is the rigorous definition of the entropy functional for systems with continuous probability. In order to proceed rigorously, one can first assume that phase space can be divided in small cells of volume  $\Delta^{(i)}$  so that the coordinates in cell  $i$  are denoted by  $x^{(i)}$ . In this manner, phase space is effectively discretized and so does the distribution function:  $\rho(x^{(i)}) \equiv \rho^{(i)}$ . The absolute information entropy can be defined as<sup>21,26</sup> as

$$S[\rho] = -k_B \sum_i \rho^{(i)} \ln \rho^{(i)}, \quad (15)$$

where  $k_B$  is Boltzmann's constant. In order to obtain the continuous limit, which is what one needs, it is not possible to perform naively the limit

$$S_{naive}[\rho] = \lim_{\Delta^{(i)} \rightarrow 0} \left( -k_B \sum_i \rho^{(i)} \ln \rho^{(i)} \right), \quad (16)$$

because this limit diverges. If one subtract the divergent contribution  $-k \ln \Delta^{(i)}$  a finite expression is obtained

$$S'_{naive}[\rho] = \int dx \rho(x) \ln \rho(x). \quad (17)$$

However, as discussed in Ref.<sup>19–21</sup>, the definition of Eq. (17) is not acceptable because it is not coordinate independent. More explicitly, it is coordinate independent only if one uses canonical coordinates (because the Jacobian of the transformation between canonical coordinates is 1). This restriction has no physical motivation. Actually, non-canonical coordinates are often more physically compelling<sup>15</sup>. For the above reasons, when studying continuous probability distributions, one must resort to the use of the relative entropy, which measure the information relative to a state of ignorance represented by a given distribution function<sup>21</sup>. If one denotes this latter distribution by  $\mu(x)$ , the relative entropy is defined by

$$S_{rel}[\rho] = -k_B \int dx \rho(x) \ln \left( \frac{\rho(x)}{\mu(x)} \right). \quad (18)$$

For canonical Hamiltonian systems, a convenient distribution function with respect to which defining the relative entropy is given by that representing the state of absolute ignorance, i.e. the uniform distribution. Then one can set  $\mu(x) = 1$  so that in practice  $S_{rel}[\rho]$  in Eq. (18) coincides with the absolute entropy  $S'_{naive}[\rho]$  in Eq. (17). However, it must be realized that a uniform distribution in canonical coordinates does not necessarily transform into another uniform distribution if more general coordinates (for example non-canonical) are used. The integral in Eq. (18) is well defined and its value does not depend from the particular coordinate choice. For example, considering the transformation  $x \rightarrow y$ , one has

$$\int dx \rho(x) \ln \left( \frac{\rho(x)}{\mu(x)} \right) = \int dy \rho'(y) \ln \left( \frac{\rho'(y)}{\mu'(y)} \right), \quad (19)$$

where  $dx \rho(x) = dy \rho'(y)$  and  $dx \mu(x) = dy \mu'(y)$ . The relative entropy  $S_{rel}[\rho]$  in Eq. (18) is a measure of negative information and it can be used as the starting point of a maximum entropy principle in order to obtain the form of the least biased or maximum non-committal distribution function  $\rho(x)$ . To this end considering, for example, the two statistical constraints  $\langle \mathcal{H} \rangle = E$  and  $\int dx \rho(x) = 1$ , obeyed by the distribution function  $\rho(x)$ , one is led to consider the quantity

$$\mathcal{I} = S_{rel}[\rho] + \lambda(E - \langle \mathcal{H} \rangle) + \gamma \left( 1 - \int dx \rho(x) \right), \quad (20)$$

where the two Lagrangian multipliers  $\lambda$  and  $\gamma$  have been introduced. If one maximizes  $\mathcal{I}$  with respecting to  $\rho(x)$ , by setting  $\delta \mathcal{I} / \delta \rho = 0$ , and eliminates the Lagrangian multiplier  $\gamma$ , the following expression for  $\rho(x)$  is easily found

$$\rho(x) = Z^{-1} \mu(x) \exp \left[ -\frac{\lambda}{k_B} \mathcal{H}(x) \right], \quad (21)$$

where  $Z = \int dx \mu(x) \exp[-(\lambda/k_B) \mathcal{H}(x)]$ . Equation (21) generalizes to the relative entropy of continuous probability distributions the standard maximum entropy principle<sup>26</sup>. In the canonical Hamiltonian case, which has been treated in this section,  $\mu(x)$  is trivially the uniform distribution. However, for non-canonical and non-Hamiltonian phase space  $\mu(x)$  plays a fundamental role.

### III. NON-CANONICAL HAMILTONIAN PHASE SPACE

Consider a transformation of phase space coordinates  $z = z(x)$  such that the Jacobian

$$\mathcal{J} = \left\| \frac{\partial x}{\partial z} \right\| \neq 1. \quad (22)$$

Coordinates  $z$  are called non-canonical. The Hamiltonian transforms as a scalar  $\mathcal{H}(x(z)) = \mathcal{H}'(z)$  and the equations of motion becomes<sup>13,15</sup>

$$\dot{z}_m = \sum_{k=1}^{2n} \mathcal{B}_{mk}(z) \frac{\partial \mathcal{H}'(z)}{\partial z_k}, \quad (23)$$

where

$$\mathcal{B}_{mk} = \sum_{i,j=1}^{2n} \frac{\partial z_m}{\partial x_i} \mathcal{B}_{ij}^s \frac{\partial z_k}{\partial x_j}. \quad (24)$$

Equations of motion can also be obtained by means of the variational principle<sup>24</sup> which arises when applying the non-canonical transformation of coordinates to the symplectic expression of the action given in Eq. (3). One obtains the following form for the action in non-canonical coordinates<sup>24</sup>

$$\mathcal{A} = \int dt \left[ \frac{1}{2} \sum_{i,j,m=1}^{2n} \frac{\partial x_i}{\partial z_m} \dot{z}_m \mathcal{B}_{ij}^s x_j(z) - \mathcal{H}'(z) \right], \quad (25)$$

on which the variation is to be performed on the  $z$  coordinates in order to obtain Eqs. (23). Poisson brackets become non-canonical brackets defined by

$$\{a', b'\} = \sum_{i,j=1}^{2n} \frac{\partial a'(z)}{\partial z_i} \mathcal{B}_{ij}(z) \frac{\partial b'(z)}{\partial z_j}, \quad (26)$$

where  $a'(z) = a(x(z))$ . Non-canonical equations of motion can expressed by means of the bracket in Eq. (26) as  $\dot{z}_i = \{z_i, \mathcal{H}'(z)\}$ . With a little bit of algebra, it is easy to verify that non-canonical brackets satisfy the Jacobi relation as an identity. The Jacobi relation leads to an identity for  $\mathcal{B}(z)$  which is easily found to be

$$S_{ijk}(z) = \sum_{l=1}^{2n} \left( \mathcal{B}_{il} \frac{\partial \mathcal{B}_{jk}(z)}{\partial z_l} + \mathcal{B}_{kl} \frac{\partial \mathcal{B}_{ij}(z)}{\partial z_l} + \mathcal{B}_{jl} \frac{\partial \mathcal{B}_{ki}(z)}{\partial z_l} \right) = 0. \quad (27)$$

The non-canonical brackets of phase space coordinates are given by

$$\{z_i, z_j\} = \mathcal{B}_{ij}(z). \quad (28)$$

Writing phase space point as  $z \equiv (\xi, \zeta)$ , one can define the operators

$$\hat{T}_\xi = \{\dots, \zeta\} \delta \xi, \quad (29)$$

$$\hat{T}_\zeta = -\{\dots, \xi\} \delta \zeta, \quad (30)$$

which realizes infinitesimal translations along the axis  $\xi$  and  $\zeta$ . It is realized that the non-canonical bracket relations of Eq. (28) imply that translations along phase space axis do no longer commute in general or, in other words, phase space is curved. Notice that there is still no need to introduce a metric tensor. One just needs to define parallel transport and an affine connection. This latter is implicitly defined by means of the non-canonical brackets and the infinitesimal translation operators  $\hat{T}_\xi$  and  $\hat{T}_\zeta$ .

Non-canonical phase spaces are Hamiltonian<sup>13,15</sup>. They are obtained by means of non-canonical transformation of coordinates applied to canonical Hamiltonian systems. Suppose that there is a system with a non-canonical bracket satisfying the Jacobi relation, or its equivalent form given in Eq. (27). Suppose also that  $\det \mathcal{B} \neq 0$ , then by Darboux's theorem the system can be put (at least locally) in canonical form. One would classify such a system as Hamiltonian. The validity of the Jacobi relation is the essence of what it means to be Hamiltonian<sup>13,15</sup>. In other words, if the algebra of brackets is a Lie algebra then phase space is Hamiltonian<sup>15</sup>. At this point, it is clear that the claim of Ref.<sup>9</sup> that non-Hamiltonian brackets can satisfy the Jacobi relation is an oxymoron (i.e. a self-contradicting assertion) and that, in reality, the work of Ref.<sup>9</sup> deals with non-canonical Hamiltonian brackets, which indeed satisfy the Jacobi relation.

For non-canonical systems, statistical mechanical averages can be calculated as

$$\langle a'(z) \rangle = \int dz \rho(z) a'(z(t)), \quad (31)$$

where

$$\rho(z) = \mathcal{J}(z) f'(z), \quad (32)$$

with the Jacobian  $\mathcal{J}(z)$  defined in Eq. (22). The Liouville operator is defined by means of the non-canonical bracket

$$iL' = \{\dots, \mathcal{H}'(z)\}, \quad (33)$$

and so time propagation is given by

$$\begin{aligned} a'(z(t)) &= \exp[itL'] a'(z) \\ &= \exp[it\{\dots, \mathcal{H}'(z)\}] a'(z). \end{aligned} \quad (34)$$

In non-canonical coordinates a compressibility

$$\kappa(z) = \sum_{i,j=1}^{2n} \frac{\partial \mathcal{B}_{ij}(z)}{\partial z_i} \frac{\partial \mathcal{H}'(z)}{\partial z_j} \quad (35)$$

might (but not necessarily) be present. See Appendix A for a simple example of a non-canonical system with zero compressibility. Integrating by parts Eq. (31), one obtains

$$\langle a'(z) \rangle = \int dz a'(z) \exp[-t(iL' + \kappa(z))] \rho(z). \quad (36)$$

Equation (36) implies that  $\rho(z)$  obeys the non-canonical Liouville equation

$$\begin{aligned} \frac{\partial \rho(z)}{\partial t} &= -(iL' + \kappa(z)) \rho(z) \\ &= \sum_{i=1}^{2n} \frac{\partial}{\partial z_i} (\dot{z}_i \rho(z)). \end{aligned} \quad (37)$$

It is easy to see that  $d\mathcal{M}(z) = \mathcal{J}(z) dz$  provides the correct invariant measure<sup>24</sup>

$$\begin{aligned} dz(t) \left\| \frac{\partial x(t)}{\partial z(t)} \right\| &= \left\| \frac{\partial z(t)}{\partial z(0)} \right\| dz(0) \left\| \frac{\partial x(t)}{\partial x(0)} \right\| \left\| \frac{\partial x(0)}{\partial z(0)} \right\| \\ &= dz(0) \left\| \frac{\partial x(0)}{\partial z(0)} \right\|, \end{aligned} \quad (38)$$

where it has been used the fact that the phase space flow in the  $x$  coordinates is canonical so that  $\|\partial x(t)/\partial x(0)\| = 1$ . The use of the Jacobian provides the correct way of defining the invariant measure because it can also be applied when there is no compressibility<sup>24</sup>. Instead, 'metric' theories<sup>7-9</sup> are useless when  $\kappa(z) = 0$ . However, as far the calculation of averages, correlation functions and linear response theory is concerned, there is hardly no need for writing the invariant measure explicitly. Knowledge of  $\rho(z)$  is just what is needed for statistical mechanics even in the non-Hamiltonian case and in the presence of constraints, as shown in Refs.<sup>6,10,11</sup>.

From the discussions given in Refs.<sup>7</sup> it would seem (incorrectly) that one would need the explicit knowledge of the Jacobian  $\mathcal{J}$  or of the 'metric' factor  $\exp[-w]$ , where  $w = \int dz \kappa(z)$ , in order to write a coordinate-independent entropy functional as

$$\begin{aligned} S_{\mathcal{J}} &= -k_B \int dz \mathcal{J}(z) f'(z) \ln f'(z) \\ &= -k_B \int dz \rho(z) \ln \left( \frac{\rho(z)}{\mathcal{J}(z)} \right). \end{aligned} \quad (39)$$

However, from the discussion of the previous section one knows that, for continuous probability distributions, the correct entropy functional is given by the relative entropy. Therefore, one just needs to transform in non-canonical coordinates Eq. (18). In non-canonical coordinates

$$\mu(x) dx = 1 \cdot dx = \mathcal{J}(z) dz \quad (40)$$

$$f(x) dx = f'(z) \mathcal{J}(z) dz = \rho(z) dz. \quad (41)$$

so that the correct definition  $S_{rel}[\rho] = -k_B \int dz \rho(z) \ln(\rho(z)/\mathcal{J}(z))$  is naturally obtained. If the Jacobian  $\mathcal{J}(z)$  is not known, one can use any other distribution function with respect to which the entropy is calculated; i.e.  $m(x)dx = m'(z)\mathcal{J}(z)dz$ . Define  $\mu(z) = m'(z)\mathcal{J}(z)$ , in analogy with  $\rho(z) = f'(z)\mathcal{J}(z)$ . One can think of  $\mu(z)$  as the solution of a Liouville equation with different interactions. For example, if  $iL' = iL'_0 + iL'_I$ , one could define  $\mu(z)$  as the solution of

$$\frac{\partial \mu(z)}{\partial t} = -(iL'_0 + \kappa_0)\mu(z), \quad (42)$$

with  $\kappa = \kappa_0 + \kappa_I$ . The entropy determined by the additional interactions, represented by  $iL'_I$ , with respect to the state where the  $iL'_I$  are absent, is given by

$$S_{rel}[\rho|\mu] = -k_B \int dz \rho(z) \ln \left( \frac{\rho(z)}{\mu(z)} \right). \quad (43)$$

Equation (43), with the correct interpretation of the distribution function  $\mu(z)$ , provides a coordinate-invariant definition of the relative entropy which does not require knowledge either of the ‘metric’ or of the Jacobian. The maximum-entropy principle, as written in the previous section for the canonical case, also applies without major changes to the non-canonical systems. The functional to be maximized is

$$\mathcal{I} = S_{rel}[\rho|\mu] + \lambda(E - \langle \mathcal{H}'(z) \rangle) + \gamma \left( 1 - \int dz \rho(z) \right),$$

which provides, by setting  $\delta \mathcal{I} / \delta \rho(z) = 0$ , the generalized canonical distribution in non-canonical coordinates

$$\rho(z) = Z_\mu^{-1} \mu(z) \exp \left[ -\frac{\lambda}{k_B} \mathcal{H}'(z) \right]. \quad (44)$$

The quantity  $Z_\mu = \int dz \mu(z) \exp[-(\lambda/k_B)\mathcal{H}'(z)]$  is a ‘weighted’ partition function.

Therefore, it is realized that the rigorous concept of relative entropy allows one to avoid the use of the (possibly unknown) Jacobian of the transformation between canonical and non-canonical coordinates. The philosophy is that, once non-canonical equations of motion are given, the non-canonical bracket and the Liouville operator can be defined. Liouville equation for  $\rho(z)$  can be written down and statistical mechanics can follow. Relative entropy and maximum-entropy principles complete the picture.

#### IV. NON-HAMILTONIAN PHASE SPACE

In Refs.<sup>10,11</sup> it was shown how non-Hamiltonian equations of motion, brackets and statistical mechanics can be defined. One must simply keep the generalized symplectic structure of the non-canonical equations in (23) and of the non-canonical bracket in Eq. (26) and, in place of  $\mathcal{B}(z)$ , use an antisymmetric matrix  $\tilde{\mathcal{B}}(z)$  which does

not obey the tensorial transformation in Eq. (24). Once  $\tilde{\mathcal{B}}(z)$  is chosen arbitrarily, with the only constraint to be antisymmetric so that the Hamiltonian is conserved, the Jacobi relation is no longer satisfied<sup>10</sup>. When the Jacobi relation is not satisfied, one of the conditions of validity of the Darboux’s theorem fails so that the non-Hamiltonian phase space flow cannot be put in canonical form. Failure of the Jacobi relation is the definition of non-Hamiltonian algebra. References<sup>10,11</sup> already showed how to define statistical mechanics and linear response theory for non-Hamiltonian system. In particular, systems with holonomic constraints were also considered<sup>11</sup>. The formalism for non-Hamiltonian phase space curvature (i.e. the non-commutation of translations about coordinate axis), and the definition of relative entropy and maximum-entropy principles are pretty similar to those of the non-canonical Hamiltonian case. In practice, as written above, one can take the results of the previous section, change  $\mathcal{B}(z)$  with  $\tilde{\mathcal{B}}(z)$  and the theory for non-Hamiltonian phase space, together with its statistical mechanics and maximum relative entropy principle, is written down. Again ‘metric’ theories of non-Hamiltonian phase space are not complete because there could be non-Hamiltonian phase space flows (i.e. flows defined by brackets which do not satisfy the Jacobi relation) with a zero compressibility. See Appendix B for an example. In order to show how this is theoretically possible, one can consider a particular sub-ensemble of non-Hamiltonian phase space flows: those that can be derived by means of a non-integrable scaling of time. Interestingly enough, it was Nosé who considered originally this kind of flows when he introduced his famous thermostat<sup>2,4</sup>. Nosé started from a canonical Hamiltonian system, performed a non-canonical transformations, and finally a non-integrable scaling of time. So it is done in the following. Consider the non-integrable scaling of time

$$dt = \Phi(z)d\tau, \quad (45)$$

where  $\tau$  is an auxiliary time variable. This scaling of  $dt$  is clearly non-integrable because, due to the dependence of  $dt$  from phase space coordinates, the integral  $\int dt$  depends from the path in phase space. If one now applies this scaling to Eq. (23), which have already been obtained by applying a non-canonical transformation to a canonical system, the following non-Hamiltonian equations are derived

$$\begin{aligned} \tilde{z}_i &= \sum_{j=1}^{2n} \Phi(z) \mathcal{B}_{ij}(z) \frac{\partial \mathcal{H}'(z)}{\partial z_j} \\ &= \sum_{j=1}^{2n} \tilde{\mathcal{B}}_{ij}(z) \frac{\partial \mathcal{H}'(z)}{\partial z_j}, \end{aligned} \quad (46)$$

where  $\tilde{z} = dz/d\tau$  and the matrix  $\tilde{\mathcal{B}}$  has been defined. From Equations (46) it is clear that in order to obtain non-Hamiltonian flows, one changes the dynamics without affecting the ‘geometric’ definition of the coordinates

in phase space. Using the antisymmetric matrix  $\tilde{\mathcal{B}}$  defined in Eq. (46), one can introduce a non-Hamiltonian bracket

$$(a', b') = \sum_{i,j=1}^{2n} \frac{\partial a'}{\partial z_i} \tilde{\mathcal{B}}_{ij}(z) \frac{\partial b'}{\partial z_j}. \quad (47)$$

This bracket does not satisfy the Jacobi relation so that the equations of motion (46) are non-Hamiltonian. In analogy with the non-canonical case, associated with the Jacobi relation there will be a tensor

$$\begin{aligned} \tilde{s}_{ijk} = & \sum_{l=1}^{2n} \left( \tilde{\mathcal{B}}_{il}(z) \frac{\partial \tilde{\mathcal{B}}_{jk}(z)}{\partial z_l} + \tilde{\mathcal{B}}_{kl}(z) \frac{\partial \tilde{\mathcal{B}}_{ij}(z)}{\partial z_l} \right. \\ & \left. + \tilde{\mathcal{B}}_{jl}(z) \frac{\partial \tilde{\mathcal{B}}_{ki}(z)}{\partial z_l} \right) \neq 0. \end{aligned} \quad (48)$$

The compressibility of the non-Hamiltonian equations in (46) is given by

$$\begin{aligned} \tilde{\kappa}(z) &= \sum_{i=1}^{2n} \frac{\partial \tilde{z}_i}{\partial z_i} = \sum_{i,j=1}^{2n} \frac{\partial \tilde{\mathcal{B}}_{ij}}{\partial z_i} \frac{\partial \mathcal{H}'(z)}{\partial z_j} \\ &= \sum_{i=1}^{2n} \frac{\partial \Phi(z)}{\partial z_i} \dot{z}_i + \Phi(z) \kappa(z), \end{aligned} \quad (49)$$

where  $\dot{z}$  and  $\kappa$  are given by the non-canonical equations of motion before the non-integrable time-scaling. It is evident that every time one chooses  $\Phi(z)$  so that

$$\sum_{i=1}^{2n} \frac{\partial \ln \Phi(z)}{\partial z_i} \dot{z}_i = -\kappa(z). \quad (50)$$

the non-Hamiltonian flows will have zero compressibility. See the trivial example given in Appendix B.

Even if one has not changed the nature of the  $z$  coordinates spanning non-Hamiltonian phase space, by means of  $\tilde{\mathcal{B}}(z)$  one has changed the affine connection, which if non-canonical coordinates without time scaling are used is determined using  $\mathcal{B}(z)$ . Accordingly, one has a distribution function obeying

$$\begin{aligned} \frac{\partial \tilde{\rho}(z)}{\partial \tau} &= -(\tilde{\rho}, \mathcal{H}'(z)) - \tilde{\kappa}(z) \tilde{\rho} \\ &= -(i\tilde{L} + \tilde{\kappa}) \tilde{\rho}(z), \end{aligned} \quad (51)$$

where the eventual compressibility is explicitly considered. Of course, one must use the non-Hamiltonian distribution  $\tilde{\rho}(z)$  for calculating averages, correlation functions and formulating linear response theory<sup>10,11</sup>. As it could be expected, the non-Hamiltonian maximum relative entropy principle provides the following form for the generalized canonical distribution function

$$\tilde{\rho}(z) = \tilde{Z}_\mu^{-1} \tilde{\mu}(z) \exp \left[ -\frac{\lambda}{k_B} \mathcal{H}'(z) \right];, \quad (52)$$

where  $\lambda$  is a Lagrange multiplier and  $\tilde{Z}_\mu = \int dz \tilde{\mu}(z) \exp[-(\lambda/k_B) \mathcal{H}'(z)]$  is the partition function weighted by means of the non-Hamiltonian auxiliary distribution  $\tilde{\mu}(z)$ .

## V. CONCLUSIONS

The geometry of phase space is peculiar. In general, canonical coordinates (regardless of their nature) are defined on Cartesian axis. When non-canonical coordinates and/or non-Hamiltonian dynamics are considered, phase space is curved. This has the group theoretical meaning that translations along different axis do not commute. This idea of curvature is qualitative (as in topology) because, rigorously speaking, the length of the line element in phase space has no physical meaning so that there is no metric tensor. In other words, phase space is an affinely connected manifold without a metric. Antisymmetric brackets, which define a Lie algebra (in the canonical and non-canonical cases) or a non-Lie algebra (in the non-Hamiltonian case), are used to connect, by means of infinitesimal ‘contact’ transformations, nearby points of the manifold. The affinity (or the Christoffel symbols) could be introduced *via* such generalized brackets but there is still no natural way to choose a metric tensor. With respect to this, it is worth to remark that, also in generalization of gravitational theories, the Palatini’s formalism considers the metric tensor and the affinity as objects that can be varied (and thus chosen) independently from each other<sup>18</sup>.

The failure of the Jacobi relation and of Darboux’s theorem is the distinctive (and defining) feature of non-Hamiltonian dynamics. Whenever a bracket satisfies the Jacobi relation (and  $\det \tilde{\mathcal{B}} \neq 0$ ), by Darboux’s theorem, such a bracket can be put in canonical form so that the algebra (and the bracket) must be classified as Hamiltonian by all means.

The presence of a phase space compressibility is not a signature of non-canonical or non-Hamiltonian dynamics. There might be cases (and it is worth to remark that Andersen’s constant pressure dynamics<sup>1</sup> is one of these) when the compressibility is zero but the dynamics is non-canonical or non-Hamiltonian. Explicit and simple examples have been given. In such cases, so called ‘metric’ theories of statistical mechanics fail because they provide incorrectly a trivial measure of phase space volume. As shown originally by Nosé, when deriving his famous thermostat<sup>2</sup>, and in this paper, the non-canonical Jacobian contains the necessary geometrical information.

Following the work of Nosé once again<sup>2,4</sup>, it has been shown that a certain class of non-Hamiltonian phase space flows may be defined by means of a non-canonical transformation of coordinates followed by a non-integrable scaling of time. In such a case, conditions in order to obtain non-Hamiltonian flows with zero compressibility have been derived and a simple example has been given.

It has been remarked how, for continuous probability distributions, one must use the relative entropy functional in order to be rigorous. The definition of the relative entropy is naturally coordinate independent and, measuring the state of ignorance relative to another given distribution, does not require the explicit knowl-

edge of the Jacobian. A maximum-entropy principle, which applies to the constrained relative entropy, has been formulated in the canonical, non-canonical and non-Hamiltonian case. This maximum-entropy principle is particularly important for applications of non-Hamiltonian dynamics in non equilibrium thermodynamical ensembles.

Mathematical languages are powerful and there is a certain freedom in their choice. If one really wants, at least when a compressibility is present, then one can use so called ‘metric’ formalisms to address non-Hamiltonian statistical mechanics. What it cannot be denied is that statistical mechanics can be formulated by means of distributions functions without defining a fictitious metric tensor<sup>10,11</sup>. These distributions naturally arise as solutions of Liouville equations that can be written once the algebra of antisymmetric brackets is given. Within this approach there is a unique, smooth path leading from generalized equations of motion to generalized statistical mechanics. Moreover, it has been shown that the algebra of non-Hamiltonian brackets can be extended to quantum theories<sup>6</sup>. It is not clear how this can be achieved by means of Riemann geometry and ‘metric’ formalisms of statistical mechanics.

In this paper the geometry of phase space has been considered under equilibrium thermodynamic conditions. There is numerical evidence that, when the dynamics is dissipative, phase space could become fractal. If phase space distribution functions are considered with an ontological status and not as mathematical objects (which act as repositories of the observer’s knowledge), this fractal nature would be an almost insurmountable obstacle to their effective use in statistical mechanics. It is worth to remark that if this ontological status of statistical distribution functions would be taken literally then, following Kohn’s provoking point of view in his nobel lecture<sup>27</sup>, they should not be considered as “legitimate scientific objects” because the *real* distribution function of a many-body interacting system is actually incalculable (just as its wave function is) even under *simple* equilibrium thermodynamic conditions. Instead, if one looks at distribution functions from Jaynes’s perspective<sup>26</sup>, as information theoretic objects that must contain only the information that is needed to predict experimental observable properties, then it is not at all proven that distribution functions of dissipative systems must represent the fractal nature of phase space in order to allow the theoreticians to make correct predictions. Which kind of information must be taken into account and by means of which constraints this could be performed is a very subtle issue that might depend of the particular phenomenon considered and that will be addressed in future papers. Nevertheless, this paper has laid the foundation of an information theoretic approach to non-Hamiltonian system out of equilibrium by means of the maximum (relative) entropy principle. This principle is what would be needed to make rigorous the approach to non-Hamiltonian non equilibrium systems of Zhukov and Cao<sup>22</sup>.

The group theoretical approach to non-Hamiltonian statistical mechanics by means of antisymmetric brackets is already established but it is still to be fully exploited with all its potentials. Classical non equilibrium ensembles, quantum-classical dynamics, and quantum theory in general are the areas where this formalism will probably have an impact. Future works will deal with these issues.

## APPENDIX A: A NON-CANONICAL SYSTEM WITH ZERO COMPRESSIBILITY

Consider the following simple Hamiltonian

$$\mathcal{H} = \frac{p_1^2}{2} + \frac{p_2^2}{2} + \frac{1}{2}(q_1 - q_2)^2. \quad (\text{A1})$$

Canonical equations of motion can be very easily written down. Consider instead the following non-canonical transformation of coordinate  $x = (q_1, q_2, p_1, p_2) \rightarrow z = (\xi_1, \xi_2, \pi_1, \pi_2)$  defined by

$$q_1 = \xi_1 \xi_2^{-1} \quad (\text{A2})$$

$$q_2 = \xi_2 \quad (\text{A3})$$

$$p_1 = \xi_2 \pi_1 \quad (\text{A4})$$

$$p_2 = \pi_2. \quad (\text{A5})$$

By using this transformation of coordinates onto the canonical equation of motion, one obtains non-canonical equations of motion

$$\dot{\xi}_1 = \xi_1 \pi_2 \xi_2^{-1} + \xi_2^2 \pi_1 \quad (\text{A6})$$

$$\dot{\xi}_2 = \pi_2 \quad (\text{A7})$$

$$\dot{\pi}_1 = -\pi_2 \xi_2^{-1} \pi_1 + \xi_2^{-1} (\xi_2 - \xi_1 \xi_2^{-1}) \quad (\text{A8})$$

$$\dot{\pi}_2 = -(\xi_2 - \xi_1 \xi_2^{-1}). \quad (\text{A9})$$

The Hamiltonian in non-canonical coordinates is

$$\mathcal{H}'(z) = \xi_2^2 \frac{\pi_1^2}{2} + \frac{\pi_2^2}{2} + \frac{1}{2}(\xi_1 \xi_2^{-1} - \xi_2)^2. \quad (\text{A10})$$

One can calculate

$$\frac{\partial \mathcal{H}'(z)}{\partial \xi_1} = \xi_2^{-1} (\xi_1 \xi_2^{-1} - \xi_2) \quad (\text{A11})$$

$$\frac{\partial \mathcal{H}'(z)}{\partial \xi_2} = \xi_2 \pi_1^2 - (\xi_1 \xi_2^{-1} - \xi_2) (\xi_1 \xi_2^{-2} + 1) \quad (\text{A12})$$

$$\frac{\partial \mathcal{H}'(z)}{\partial \pi_1} = a \xi_2^2 \pi_1 \quad (\text{A13})$$

$$\frac{\partial \mathcal{H}'(z)}{\partial \pi_2} = \pi_2, \quad (\text{A14})$$

and write the equations in matrix form

$$\begin{bmatrix} \dot{\xi}_1 \\ \dot{\xi}_2 \\ \dot{\pi}_1 \\ \dot{\pi}_2 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & \xi_1 \xi_2^{-1} \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & -\pi_1 \xi_2^{-1} \\ -\xi_1 \xi_2^{-1} & -1 & \pi_1 \xi_2^{-1} & 0 \end{bmatrix}$$

$$\times \begin{bmatrix} \partial\mathcal{H}'(z)/\partial\xi_1 \\ \partial\mathcal{H}'(z)/\partial\xi_2 \\ \partial\mathcal{H}'(z)/\partial\pi_1 \\ \partial\mathcal{H}'(z)/\partial\pi_2 \end{bmatrix}. \quad (\text{A15})$$

Equations (A6-A10) are obviously non-canonical, as it is clearly seen by their matrix form given in Eq. (A15), and they have a zero compressibility. Because the compressibility is zero, as discussed in the previous sections, ‘metric’ theories cannot be applied. The antisymmetric matrix appearing in Eq. (A15) must be used to define the non-canonical bracket, which obviously satisfies the Jacobi relation, and the Liouville equation.

## APPENDIX B: A NON-HAMILTONIAN SYSTEM WITH ZERO COMPRESSIBILITY

Consider the Hamiltonian of Eq. (A1). First obtain non-canonical equations of motion by considering the transformation of coordinates

$$q_1 = \xi_2 \xi_1 \quad (\text{B1})$$

$$q_2 = \xi_2 \quad (\text{B2})$$

$$p_1 = \pi_1 \quad (\text{B3})$$

$$p_2 = \pi_2. \quad (\text{B4})$$

The Hamiltonian becomes

$$\mathcal{H}' = \frac{\pi_1^2}{2} + \frac{\pi_2^2}{2} + \frac{\xi_2^2}{2}(\xi_1 - 1)^2. \quad (\text{B5})$$

The non-canonical equations of motion are

$$\dot{\xi}_1 = \xi_2^{-1}\pi_1 - \xi_1\xi_2^{-1}\pi_2 \quad (\text{B6})$$

$$\dot{\xi}_2 = \pi_2 \quad (\text{B7})$$

$$\dot{\pi}_1 = -\xi_2(\xi_1 - 1) \quad (\text{B8})$$

$$\dot{\pi}_2 = -\xi_2(1 - \xi_1). \quad (\text{B9})$$

These non-canonical equations have a compressibility

$$\kappa = -\xi_2^{-1}\pi_2, \quad (\text{B10})$$

and define the antisymmetric matrix

$$\mathcal{B} = \begin{bmatrix} 0 & 0 & \xi_2^{-1} & -\xi_2^{-1}\xi_1 \\ 0 & 0 & 0 & 1 \\ -\xi_2^{-1} & 0 & 0 & 0 \\ \xi_2^{-1}\xi_1 & -1 & 0 & 0 \end{bmatrix} \quad (\text{B11})$$

which must be used in order to define the non-canonical bracket which satisfy the Jacobi relation. Now if one wants to apply a non-integrable scaling of time in order to obtain a non-Hamiltonian flow with zero compressibility  $\tilde{\kappa}$ , Eq. (50) can be used. Assuming the scaling function  $\Phi = \Phi(\xi_2)$  one obtains

$$\frac{\partial\Phi}{\partial\xi_2}\pi_2 = \xi_2^{-1}\pi_2, \quad (\text{B12})$$

from which it is readily found  $\Phi = \xi_2$ . Then, the antisymmetric matrix  $\tilde{\mathcal{B}} = \Phi\mathcal{B}$  by means of which non-Hamiltonian brackets can be defined, is

$$\tilde{\mathcal{B}} = \begin{bmatrix} 0 & 0 & 1 & -\xi_1 \\ 0 & 0 & 0 & \xi_2 \\ -1 & 0 & 0 & 0 \\ \xi_1 & -\xi_2 & 0 & 0 \end{bmatrix}. \quad (\text{B13})$$

Non-Hamiltonian equations of motion are now defined according to Eq. (46). Finally with a little bit of algebra it is easy to verify that the non-Hamiltonian bracket of Eq. (47), with  $\tilde{\mathcal{B}}$  defined in Eq. (B13), does not satisfy the Jacobi relation and  $\tilde{S}_{ijk} \neq 0$ . For example, it is easy to verify that  $\tilde{S}_{314} = 1$ .

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