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On the statistical mechanics of non-Hamiltonian systems: the generalized Liouville equation, entropy, and time-dependent metrics

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Several questions in the statistical mechanics of non-Hamiltonian systems are discussed. The theory of differential forms on the phase space manifold is applied to provide a fully covariant formulation of the generalized Liouville equation. The properties of invariant volume elements are considered, and the nonexistence in general of smooth invariant measures noted. The time evolution of the generalized Gibbs entropy associated with a given choice of volume form is studied, and conditions under which the entropy is constant are discussed. For non-Hamiltonian systems on manifolds with a metric tensor compatible with the flow, it is shown that the associated metric factor is in general a time-dependent solution of the generalized Liouville equation.

KEY WORDS: non-Hamiltonian dynamics, ergodic theory, applied differential forms

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1. Introduction

The dynamics of Hamiltonian systems is characterized by conservation of phase space volume under time evolution [1], and this conservation of phase volume is a cornerstone of conventional statistical mechanics [2,3]. Invariance of phase space volume under Hamiltonian time evolution is the content of Liouville's theorem for divergenceless flows [1,4]. At a deeper level, conservation of phase space volume is understood to be a consequence of the existence of an invariant symplectic form in the phase space of Hamiltonian systems, and application of geometric methods and concepts from the theory of differentiable manifolds [5–9] is essential for a fundamental description of classical Hamiltonian systems [1,5,10–12].

Non-Hamiltonian dynamics, characterized by nonzero phase space compressibility [4,13–22], is relevant when we consider the statistical mechanics of thermostatted systems [23–26]. Such systems arise in the simulation of ensembles other than microcanonical [27], and in the treatment of nonequilibrium steady states [23,24,26,28].

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Various homogeneous thermostatting mechanisms have been introduced to remove heat supplied by nonequilibrium mechanical and thermal perturbations [23–25,27]. Phase space volume is no longer necessarily conserved, and for nonequilibrium steady states the phase space probability distribution is found to collapse onto a fractal set of dimensionality lower than in the equilibrium case [23,24,26,29,30]. This phenomenon indicates a lack of smoothness of the invariant measure in phase space in nonequilibrium steady states [26,31,32].

The dynamical evolution of the phase space distribution function for Hamiltonian systems is described by the Liouville equation [2,3]. The Hamiltonian equation is often considered be a special case of a so-called “generalized Liouville equation” (henceforth GLE) appropriate for systems with compressible dynamics [4,13–22,33], although the equation for the time-evolution of the Jacobian determinant in a general compressible flow (cf. (2.20) below) given in Liouville’s original paper [4] is, in fact, equivalent to the GLE [17,19,21]. We shall use the term GLE in accord with common usage. A number of authors [13–22] have treated the statistical mechanics of non-Hamiltonian systems in terms of the GLE, and all have derived the result that the rate of change of the Gibbs entropy for non-Hamiltonian systems is the ensemble average of the divergence of the dynamical vector field (phase space compressibility).

Steeb [15,18,33] applied the theory of Lie derivatives and differential forms to derive the GLE for both time-independent and time-dependent vector fields. Some explicit solutions to the Liouville equation were given, and the existence of singular solutions for systems with limit cycles (attracting periodic orbits) was noted [18].

The important paper by Ramshaw [22] gave a covariant formulation of the Liouville equation and of the entropy. It was noted that invariant measures (volume elements) associated with zero entropy production rate in non-Hamiltonian systems must be smooth stationary solutions of the GLE.

Some limitations of the description of nonequilibrium steady states in terms of the GLE were discussed by Holian et al. [34].

Tuckerman et al. [43] (hereafter, TEA) have recently applied geometric methods from the theory of differentiable manifolds [6–9], in particular the concepts of Riemannian geometry [8], to the classical statistical mechanics of non-Hamiltonian systems [35–37]. TEA have argued that, through introduction of so-called metric factors, it is always possible to define a smooth invariant phase space measure in non-Hamiltonian systems, even for nonequilibrium stationary states [35,36]. Moreover, the Gibbs entropy of the associated phase space distribution function is found to be constant in time, just as for Hamiltonian systems. TEA also claim that previous formulations of the GLE (for example, papers [23,24]) are in some way incorrect, incomplete, or at least coordinate-dependent [35–37]. These claims have proved controversial [38–46].

In the present paper we consider a number of questions in the statistical mechanics of non-Hamiltonian systems raised in [35–37], with particular emphasis on a coordinate-free formulation of the problem [18]. By definition, a coordinate-free formulation in the language of differential forms [5–9] removes any question [37] concerning the coordinate dependence of any results obtained. The apparatus of differential forms is the appropriate machinery for treating the transformations of variables and volume elements arising in the dynamics of both Hamiltonian and non-Hamiltonian systems.

The present paper is organized as follows. Section 2 introduces our notation for the basic objects from the theory of vector fields and differential forms [5–9]. In section 3 we review the transport (continuity) equation [6,7,18], which is the fundamental equation governing the evolution of the representative ensemble in phase space. The basic object under consideration is the density n-form ρ [6,7], which describes the phase space probability distribution. For any region of phase space, the fraction of the ensemble inside the region is obtained by integration of the density n-form over the region. The density n-form can be written as the product of a volume form [6,7] (comoving volume element) and a phase space distribution function. The GLE, which describes the evolution of the phase space distribution function, then follows from the transport equation [18]. To determine the fraction of the ensemble in a given region, we simply need to count ensemble members. As we do not need a volume form to count ensemble members inside a prescribed region of phase space, the density n-form ρ is defined without reference to any particular volume form. Any result expressed in terms of ρ alone is therefore manifestly independent of the choice of volume form on the phase space manifold. This covariance with respect to the choice of volume form is the essential advantage of a description of the ensemble density in terms of the n-form ρ.

When considering the phase space structure and dynamics of Hamiltonian and non-Hamiltonian systems, the notion of distance associated with the familiar properties of Riemannian manifolds [6] is irrelevant. Volume forms provide exactly the construct needed, namely, a definition of "volume without distance". Moreover, the Lie derivative of the volume form provides a definition of "divergence without metric connection".

Section 4 discusses in more detail the properties of invariant volume forms (invariant measures) in non-Hamiltonian systems. The existence of an invariant volume form is important for simulation of equilibrium properties via non-Hamiltonian dynamics; if the dynamics preserves a given volume form (invariant measure) then, provided the system is ergodic, and that all relevant constraints are taken into account [37], phase space averages with respect to the invariant measure can be evaluated by computing long-time averages over a single trajectory. We point out that invariant volume forms in phase space must by definition be time-independent, and conditions for the existence of smooth, stationary invariant measures are examined. For all the *equilibrium* non-Hamiltonian systems discussed to date, a smooth stationary invariant measure can be found [37]. Nevertheless, any system with *net* attracting or repelling periodic orbits cannot possess a smooth invariant measure [47], so that, contrary to the assumption made in [36], smooth invariant measures for arbitrary non-Hamiltonian systems do not exist. We then discuss a proposed time-dependent generalization of the concept of invariant measure [37], which involves a volume form that itself satisfies the GLE. True invariant measures, which are in general singular (not absolutely continuous with respect to the usual volume element), can be defined in terms of infinite-time averages of the density n-form ρ_t [32].

In section 5, we examine the time evolution of the Gibbs entropy associated with a given volume form. Several special cases are considered; in particular, the entropy is constant when the volume form satisfies the transport equation [37,48]. We discuss the significance of this result, taking careful note of the essential distinction between the coordinate-independence of the expression for the entropy and the dependence of the value of the entropy on the chosen volume form.

Our considerations up to this point make no use of any metric tensor or Riemannian structure in phase space. The implications of the existence of a phase space metric tensor are examined in section 6. It is shown that, if the metric tensor is stationary, then compatibility of the Riemannian structure with the dynamics requires the associated metric factor $\sqrt{g}$ to be a time-independent solution of the GLE. In this case, the metric factor defines an invariant (Riemannian) volume form in the usual fashion [6]. On the other hand, if the metric tensor is allowed to be time-dependent [37,49,50], then compatibility requires the associated metric factor to be a non-stationary solution of the Liouville equation. The entropy defined with respect to the associated time-dependent Riemannian volume form is then constant [37]; for nonequilibrium steady states, the underlying metric factor will become ever more nearly singular ("fractal") at long times, so that this result is only of formal significance. Section 7 concludes.

After the work reported here was completed, we received a preprint of the paper by Ramshaw [46]. Despite the rather different approach taken, the conclusions reached in our own work concerning the work of TEA are in accord with those of Ramshaw. We also note the very recent work of Sergi [51] (see also [52]), in which non-Hamiltonian statistical mechanics is discussed in terms of a generalized bracket structure. Sergi also discusses the significance of metric structure in phase space.

2. Definitions and notation

In this section we briefly review some concepts from the theory of vector fields and forms on manifolds. The discussion here is only intended to establish notation; some standard texts are [5–9].

The n-dimensional differentiable manifold of interest (phase space) is denoted $\mathcal{M}$. Coordinates are $\boldsymbol{x} = (x^1, \ldots, x^n)$. An example with $n = 2N$ is the phase space of a Hamiltonian system, with $2N$ canonical coordinates $(p_1, \ldots, p_N, q^1, \ldots, q^N)$. Such a manifold has a natural symplectic structure (2-form) preserved by the Hamiltonian flow [1]. We do not assume the existence of such Hamiltonian structure. All results concerning the GLE and entropy, etc., are moreover derived without assuming the existence of a metric tensor, either time-independent or time-dependent, on the manifold $\mathcal{M}$. Phase space is therefore not assumed to be a Riemannian manifold. (Note that the study of the Riemannian geometry of *configuration space* has yielded fundamental insights into the onset of global stochasticity in multidimensional Hamiltonian systems [53,54].) In the treatment of homogeneously thermostatted systems, the set of coordinates $\boldsymbol{x}$ consists of the position and momentum coordinates of the physical system augmented by a set of extra variables describing the thermostat [23–25,27].

The dynamics is described by a smooth vector field $\boldsymbol{\xi}(\boldsymbol{x})$,

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{\xi}, \tag{2.1}$$

with components ξ^i in basis $\partial/\partial x^i$. For simplicity, we consider the case where the vector field $\boldsymbol{\xi}$ is time-independent; a geometrical approach to response in time-dependent fields has been given elsewhere [55]. The associated evolution operator or flow ϕ_t maps the point $\boldsymbol{x} \in \mathcal{M}$ at (arbitrary) time s to the point $\phi_t \boldsymbol{x} \in \mathcal{M}$ at time $s + t$:

$$\phi_t : \boldsymbol{x} \mapsto \phi_t \boldsymbol{x}. \tag{2.2}$$

The $\{\phi_t\}$ are assumed to form a one-parameter family of diffeomorphisms of $\mathcal{M}$ onto itself.

The concept of the volume n-form is of central importance in discussions of the GLE and related questions [15]. The standard volume n-form (volume element) associated with the set of phase space coordinates $\boldsymbol{x}$ is the n-fold exterior product $\omega \equiv \omega_{\boldsymbol{x}}$

$$\omega = \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \cdots \wedge \mathrm{d}x^n. \tag{2.3}$$

The number $\omega(\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_n)$ is by definition the volume of the parallelepiped spanned by the n tangent vectors $(\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_n)$ at $\boldsymbol{x}$. The volume n-form $\bar{\omega}$ is defined by multiplying the standard volume form ω by a nonzero, smooth function $\bar{\sigma}(\boldsymbol{x})$,

$$\bar{\omega} \equiv \bar{\sigma}(\boldsymbol{x})\omega = \bar{\sigma}(\boldsymbol{x})\, \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \cdots \wedge \mathrm{d}x^n. \tag{2.4}$$

The induced action of the flow ϕ_t on a vector field $\boldsymbol{v}$ is described by the derivative map $\phi_{t*} : \boldsymbol{v} \mapsto \phi_{t*}\boldsymbol{v}$, where the "pushed forward" vector $\phi_{t*}\boldsymbol{v} \in T_{\phi_t \boldsymbol{x}}\mathcal{M}$ has components $v^i M(\phi_t \boldsymbol{x}; \boldsymbol{x})_i^j$, where $M(\phi_t \boldsymbol{x}; \boldsymbol{x})_i^j$ is the dynamical stability matrix [56].

The *pull-back* of the time-independent function $B = B(\boldsymbol{x})$ under the mapping ϕ_t is the function $\phi_t^* B$, where

$$\phi_t^* B(\boldsymbol{x}) \equiv B\big(\phi_t(\boldsymbol{x})\big). \tag{2.5}$$

The pull-back $\phi_t^* \boldsymbol{\alpha}$ of a p-form $\boldsymbol{\alpha}$ is defined by

$$\phi_t^* \boldsymbol{\alpha}\big|_{\boldsymbol{x}}(\boldsymbol{v}_1, \ldots, \boldsymbol{v}_p) = \boldsymbol{\alpha}\big|_{\phi_t \boldsymbol{x}}(\phi_{t*}\boldsymbol{v}_1, \ldots, \phi_{t*}\boldsymbol{v}_p). \tag{2.6}$$

Note that the form $\phi_t^* \boldsymbol{\alpha}$ acts on tangent vectors at the point $\boldsymbol{x}$, information on the form $\boldsymbol{\alpha}$ and tangent vectors $\phi_{t*}\boldsymbol{v}$ at the evolved point $\phi_t \boldsymbol{x}$ having been "pulled back" to the initial point $\boldsymbol{x}$ (cf. [34]).

The pull-back of the volume form ω, $\phi_t^* \omega$, is of particular significance in the statistical mechanics of Hamiltonian and non-Hamiltonian systems. The quantity $\phi_t^* \omega(\phi_{t*}\boldsymbol{v}_1, \ldots, \phi_{t*}\boldsymbol{v}_n)$ is the volume of the parallelepiped spanned by the n time-evolved tangent vectors $\{\phi_{t*}\boldsymbol{v}_1, \ldots, \phi_{t*}\boldsymbol{v}_n\}$ at the point $\phi_t \boldsymbol{x}$. Evaluation of $\phi_t^* \omega$ using (2.3) and (2.6) shows that

$$\phi_t^* \omega \equiv J_\omega(\phi_t)\omega, \tag{2.7}$$

where $J_\omega(\phi_t)(\boldsymbol{x}) = \det|\partial\phi_t\boldsymbol{x}/\partial\boldsymbol{x}|$ is the determinant of the dynamical stability matrix, that is, the Jacobian for the transformation (2.2). Obviously, $J_\omega(\phi_{t=0}) = 1$ for all $\boldsymbol{x}$. For Hamiltonian dynamics, the Jacobian is unity for all t, and the volume form is invariant under the flow, $\phi_t^*\omega = \omega$ [1]; this is one statement of Liouville's theorem for Hamiltonian systems. For non-Hamiltonian systems, the value of the Jacobian determines the growth or shrinkage of the comoving volume element along the dynamical trajectory from $\boldsymbol{x}$ at time s to $\phi_t\boldsymbol{x}$ at time t [41].

The pull-back of the generalized volume n-form $\bar{\omega}$ is [7, 6.5.12]

$$\phi_t^*\bar{\omega} \equiv J_{\bar{\omega}}(\phi_t)\bar{\omega} = \left|\frac{\partial\phi_t\boldsymbol{x}}{\partial\boldsymbol{x}}\right|\frac{\bar{\sigma}(\phi_t\boldsymbol{x})}{\bar{\sigma}(\boldsymbol{x})}\bar{\omega}. \tag{2.8}$$

For the case of a time-independent vector field $\boldsymbol{\xi}$, the result (2.8) shows that, *if* a function $\bar{\sigma}(\boldsymbol{x})$ can be found such that

$$\frac{\bar{\sigma}(\phi_t\boldsymbol{x})}{\bar{\sigma}(\boldsymbol{x})} = \left|\frac{\partial\phi_t\boldsymbol{x}}{\partial\boldsymbol{x}}\right|^{-1} \tag{2.9}$$

for all $\boldsymbol{x}$ and t, then the volume form $\bar{\omega}$ is invariant under the flow ϕ_t (cf. section 4).

The Lie derivative $\mathcal{L}_{\boldsymbol{\xi}}$ of a function B along the vector field $\boldsymbol{\xi}$ is defined by

$$\mathcal{L}_{\boldsymbol{\xi}}B = \frac{\mathrm{d}}{\mathrm{d}\tau}\phi_\tau^*B\bigg|_{\tau=0}. \tag{2.10}$$

From the definition, $\mathcal{L}$ is the differential operator (cf. the usual Liouvillian operator [23])

$$\mathcal{L} \equiv \mathcal{L}_{\boldsymbol{\xi}} = \xi^j(\boldsymbol{x})\frac{\partial}{\partial x^j}. \tag{2.11}$$

The Lie derivative of a form $\boldsymbol{\alpha}$ is defined similarly, either via

$$\mathcal{L}\boldsymbol{\alpha} = \frac{\mathrm{d}}{\mathrm{d}\tau}\phi_\tau^*\boldsymbol{\alpha}\bigg|_{\tau=0} \tag{2.12}$$

or through Cartan's formula [6,9]

$$\mathcal{L}\boldsymbol{\alpha} = i_{\boldsymbol{\xi}}\mathrm{d}\boldsymbol{\alpha} + \mathrm{d}i_{\boldsymbol{\xi}}\boldsymbol{\alpha}, \tag{2.13}$$

where d is the exterior derivative [6,9] and $i_{\boldsymbol{\xi}}\boldsymbol{\alpha}$ is the interior product (contraction) of the form $\boldsymbol{\alpha}$ with the vector $\boldsymbol{\xi}$ [6,9]. We have [7, 5.4.5]

$$\frac{\mathrm{d}}{\mathrm{d}t}\phi_t^*\boldsymbol{\alpha}_t = \phi_t^*\left[\mathcal{L}\boldsymbol{\alpha}_t + \frac{\partial\boldsymbol{\alpha}_t}{\partial t}\right]. \tag{2.14}$$

The ω-divergence $\mathrm{div}_\omega\boldsymbol{\xi}$ of the vector field $\boldsymbol{\xi}$ [6,7] is defined by the action of the Lie derivative on the n-form ω:

$$\mathcal{L}\omega = (\mathrm{div}_\omega\boldsymbol{\xi})\omega. \tag{2.15}$$

The ω-divergence is independent of coordinate system; using the definitions above, in terms of coordinates $\boldsymbol{x}$ it is

$$\text{div}_\omega(\boldsymbol{\xi}) = \frac{\partial}{\partial x^j}\big(\xi^j(\boldsymbol{x})\big). \tag{2.16}$$

The definition of the ω-divergence does not depend in any way on the existence of a metric tensor on $\mathcal{M}$. The $\bar{\omega}$-divergence is defined similarly:

$$\mathcal{L}\bar{\omega} = (\text{div}_{\bar{\omega}}\boldsymbol{\xi})\bar{\omega}, \tag{2.17}$$

with

$$\text{div}_{\bar{\omega}}\boldsymbol{\xi} = \frac{1}{\bar{\sigma}(\boldsymbol{x})}\frac{\partial}{\partial x^j}\big(\bar{\sigma}(\boldsymbol{x})\xi^j(\boldsymbol{x})\big). \tag{2.18}$$

If the form $\boldsymbol{\alpha}$ is invariant under the flow, $\phi_t^*\boldsymbol{\alpha} = \boldsymbol{\alpha}$, then from (2.12) $\mathcal{L}\boldsymbol{\alpha} = 0$. The condition that the n-form $\bar{\omega} = \bar{\sigma}(\boldsymbol{x})\omega$ be invariant under the flow is therefore (cf. section 4)

$$\text{div}_\omega\big(\bar{\sigma}\boldsymbol{\xi}\big) = 0. \tag{2.19}$$

Using equations (2.7), (2.14) and (2.15), we obtain the equation of motion for the Jacobian $J_\omega(\phi_t)$ [4]:

$$\frac{\mathrm{d}}{\mathrm{d}t}\ln J_\omega(\phi_t)(\boldsymbol{x}) = \text{div}_\omega\big(\boldsymbol{\xi}(\phi_t\boldsymbol{x})\big) \tag{2.20a}$$

$$= \kappa(\phi_t\boldsymbol{x}), \tag{2.20b}$$

where the *phase space compressibility*, $\kappa(\boldsymbol{x})$, is defined as

$$\kappa(\boldsymbol{x}) \equiv \text{div}_\omega\big(\boldsymbol{\xi}(\boldsymbol{x})\big) = \frac{\partial}{\partial x^j}\xi^j(\boldsymbol{x}). \tag{2.21}$$

For incompressible flow (e.g., Hamiltonian case), the phase space compressibility $\kappa = 0$, so that the Jacobian is always unity. In the general case, equation (2.20) can be formally solved to yield

$$J_\omega(\phi_t)(\boldsymbol{x}) = \exp\left[\int_0^t \mathrm{d}\tau\,\kappa(\phi_\tau\boldsymbol{x})\right]. \tag{2.22}$$

3. Time-dependent forms and the transport (continuity) equation

The time-dependent density n-form ρ_t is defined such that the fraction of the representative ensemble contained in any n-dimensional phase space region $\mathcal{R} \subseteq \mathcal{M}$ at time t is obtained by integrating the n-form ρ_t over the region $\mathcal{R}$ [7],

$$F_t(\mathcal{R}) = \int_{\mathcal{R}} \rho_t. \tag{3.1}$$

The normalization condition is

$$\int_{\mathcal{M}} \rho_t = 1 \tag{3.2}$$

for all t, where the integral extends over the whole phase space $\mathcal{M}$. The density n-form ρ_t provides the fundamental mathematical description of the ensemble phase space distribution. To calculate the probability $F_t(\mathcal{R})$ associated with a particular region $\mathcal{R}$, we need only (in principle) count the ensemble members within $\mathcal{R}$; the definition of ρ_t is therefore independent of any choice of volume form on $\mathcal{M}$.

An essential physical requirement is conservation of ensemble members under time evolution ϕ_t:

$$F_{t=0}(\mathcal{R}) = F_t(\phi_t\mathcal{R}), \tag{3.3a}$$

or

$$\int_{\mathcal{R}} \rho_0 = \int_{\phi_t\mathcal{R}} \rho_t, \tag{3.3b}$$

where region $\mathcal{R}$ at time $t = 0$ evolves into region $\phi_t\mathcal{R}$ at time t under the action of the flow. The pull-back of the density n-form ρ_t, $\phi_t^*\rho_t$, satisfies [7, 7.1.2]

$$\int_{\mathcal{R}} \phi_t^*\rho_t = \int_{\phi_t\mathcal{R}} \rho_t, \tag{3.4}$$

so that conservation of ensemble members is equivalent to the condition

$$\phi_t^*\rho_t = \rho_0 \tag{3.5}$$

(almost everywhere). Differentiation of both sides of (3.5) with respect to t and use of (2.14) yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\phi_t^*\rho_t = \phi_t^*\left[\frac{\partial\rho_t}{\partial t} + \mathcal{L}\rho_t\right] = 0, \tag{3.6}$$

which leads to the fundamental transport/continuity equation for the n-form ρ_t [7, 7.1B]:

$$\frac{\partial\rho_t}{\partial t} + \mathcal{L}\rho_t = 0. \tag{3.7}$$

Equation (3.7) is the basic relation governing the evolution of the ensemble density in phase space. As it is expressed in terms of the n-form ρ_t, the transport equation is completely coordinate-independent, and, moreover, does not depend in any way on a particular choice of volume form $\bar{\omega}$ on $\mathcal{M}$.

In terms of the standard volume form (2.3) we write the density n-form as

$$\rho_t \equiv f(t, \boldsymbol{x})\omega \equiv f_t\omega, \tag{3.8}$$

where $f(t, \boldsymbol{x})$ is the corresponding phase space distribution function. From equation (3.7), we have

$$\left[\frac{\partial f}{\partial t} + \mathcal{L} f + f \mathrm{div}_\omega(\boldsymbol{\xi})\right]\omega = \left[\frac{\partial f}{\partial t} + \mathrm{div}_\omega(f\boldsymbol{\xi})\right]\omega = 0, \tag{3.9}$$

which yields the GLE for f

$$\frac{\partial f}{\partial t} + \mathcal{L} f + f\kappa = \frac{\partial f}{\partial t} + \mathrm{div}_\omega(f\boldsymbol{\xi}) = 0. \tag{3.10}$$

Equation (3.10) is the covariant form of the Liouville equation for non-Hamiltonian systems [15]. It holds for both time-independent and time-dependent flows [15]. For Hamiltonian dynamics,

$$\frac{\partial f}{\partial t} + \mathrm{div}_\omega(f\boldsymbol{\xi}) = \frac{\partial f}{\partial t} + \mathcal{L} f = \frac{\mathrm{d}f}{\mathrm{d}t} = 0, \tag{3.11}$$

so that the phase space distribution function f is a time-dependent constant of the motion [57].

The GLE (3.10) is written in a manifestly coordinate-free fashion, and does not depend in any way on the particular coordinate system in which calculations are carried out [37]. The standard volume form ω (2.3) is nevertheless associated in a natural way with the particular set of coordinates $\boldsymbol{x} = (x^1, \dots, x^n)$, so that, as our notation makes clear, the actual Liouville equation (3.10) satisfied by the function f does depend on the volume form ω with respect to which the divergence of $\boldsymbol{\xi}$ is evaluated. A different choice of volume form, $\bar{\omega}$, will lead to a different decomposition of the n-form ρ_t,

$$\rho_t = \bar{f}_t \bar{\omega}. \tag{3.12}$$

Although f and $\bar{f}$ are different functions, the n-form ρ_t is completely indifferent to the choice of volume form on $\mathcal{M}$, and any result expressed in terms of ρ_t alone is therefore also manifestly independent of the choice of volume form.

Substituting the decomposition (3.12) into the transport equation (3.7), and allowing the volume form $\bar{\omega}$ to be time-dependent, we obtain the general coupled evolution equation for $\bar{f}$ and $\bar{\omega}$:

$$\bar{f}\left[\frac{\partial \bar{\omega}}{\partial t} + \mathcal{L}\bar{\omega}\right] + \left[\frac{\partial \bar{f}}{\partial t} + \mathcal{L}\bar{f}\right]\bar{\omega} = 0. \tag{3.13}$$

There are several special cases to consider. First of all, if $\bar{\omega}$ is time-independent, $\partial_t \bar{\omega} = 0$, then the phase space distribution function $\bar{f}$ will satisfy the GLE

$$\frac{\partial \bar{f}}{\partial t} + \mathcal{L}\bar{f} + \bar{f}\mathrm{div}_{\bar{\omega}}(\boldsymbol{\xi}) = \frac{\partial \bar{f}}{\partial t} + \mathrm{div}_{\bar{\omega}}(\bar{f}\boldsymbol{\xi}) = 0, \tag{3.14}$$

which has precisely the same form as (3.10) with $\omega \leftrightarrow \bar{\omega}$, $f \leftrightarrow \bar{f}$. The formulation is therefore manifestly covariant with respect to changes in the choice of decomposition of ρ_t, and the GLEs (3.10) and (3.14) are equally valid equations for the relevant phase space distribution functions.

Next suppose that the volume n-form $\bar{\omega}$ *itself* satisfies the transport equation,

$$\frac{\partial \bar{\omega}}{\partial t} + \mathcal{L}\bar{\omega} = 0. \tag{3.15}$$

From the definition of $\bar{\omega}$, equation (2.4), the function $\bar{\sigma}$ must satisfy the *same* GLE (3.10) as that satisfied by f,

$$\frac{\partial \bar{\sigma}}{\partial t} + \mathrm{div}_\omega(\bar{\sigma}\boldsymbol{\xi}) = 0, \tag{3.16}$$

while from (3.13) we see that the associated distribution function $\bar{f}$ satisfies the Liouville equation corresponding to *incompressible* propagation of $\bar{f}$ along the flow generated by $\boldsymbol{\xi}$ [7, 8.2.1]

$$\frac{\partial \bar{f}}{\partial t} + \mathcal{L}\bar{f} = 0. \tag{3.17}$$

The proposal to use a time-dependent "metric factor" $\sqrt{g}(\boldsymbol{x}, t)$ in the volume element ([37], see section 6) corresponds precisely to finding an n-form $\bar{\omega}$ that satisfies the transport equation, equation (3.15). The method proposed for computation of $\sqrt{g}$, namely, integration of the compressibility κ along trajectories [37], corresponds to solution of the partial differential equation (3.16) for $\sqrt{g}$ (i.e., $\bar{\sigma}$) by the method of characteristics [58].

Suppose finally that, in addition to satisfying the transport equation, the n-form $\bar{\omega}$ is time-independent, $\partial_t\bar{\omega} = 0$. The volume form $\bar{\omega}$ is then *invariant*, $\mathcal{L}\bar{\omega} = 0$, and defines an invariant measure [47]. The associated function $\bar{\sigma}$ satisfies the time-independent Liouville equation

$$\mathrm{div}_\omega\big(\bar{\sigma}\boldsymbol{\xi}\big) = \mathcal{L}\bar{\sigma} + \bar{\sigma}\kappa = 0. \tag{3.18}$$

In order to obtain an invariant measure of the form $\bar{\omega} = \bar{\sigma}\omega$, it is therefore necessary to solve (3.18) for stationary $\bar{\sigma}$ [22].

4. Invariant volume forms

4.1. Time-independent invariant volume forms

We now consider in more detail the properties of stationary invariant volume forms $\bar{\omega}$. Invariance of the volume form implies that, for any phase space region $\mathcal{R} \subset \mathcal{M}$, the "size" of $\mathcal{R}$ as measured by $\bar{\omega}$ is unchanged when $\mathcal{R}$ is mapped to the region $\phi_t\mathcal{R}$ under the flow, that is,

$$\int_{\mathcal{R}} \bar{\omega} = \int_{\phi_t\mathcal{R}} \bar{\omega}. \tag{4.1}$$

Let us write the invariant volume form $\bar{\omega}$ in the form (2.4), where the density $\bar{\sigma}(\boldsymbol{x})$ is a time-independent function of $\boldsymbol{x}$. In order for $\bar{\omega}$ to be a volume form, the function $\bar{\sigma}(\boldsymbol{x})$ must be be single-valued and nonzero. There has been some discussion as to whether or not $\bar{\sigma}$ is smooth as opposed to fractal [35,44,45]. Both numerical evidence (e.g. [24, 30]) and fundamental theoretical arguments [26,32,59] point to the existence of fractal structure in the invariant measures of nonequilibrium steady states. It is nevertheless of interest to consider conditions under which we can define an invariant measure of the form (2.4), where the function $\bar{\sigma}$ is "smooth".

While previous discussions have focussed on the smoothness property of $\bar{\sigma}$ [35,44, 45], the volume form $\bar{\omega} = \bar{\sigma}\omega$ need only be absolutely continuous with respect to the standard volume form ω (Liouville measure) [60,61]. The property of absolute continuity means that, for all regions $\mathcal{R}$ whose ω-volume

$$V_{\omega}(\mathcal{R}) \equiv \int_{\mathcal{R}} \omega \tag{4.2}$$

is zero, the corresponding $\bar{\omega}$-volume $V_{\bar{\omega}}(\mathcal{R})$ is also zero [60,61]. Singular probability distributions, e.g., $\bar{\sigma} = \delta(\boldsymbol{x})$, are therefore excluded [61], but absolutely continuous densities are not necessarily either continuous or differentiable.

The invariance condition (4.1) can be written as

$$\int_{\mathcal{R}} \bar{\omega} = \int_{\mathcal{R}} \phi_t^* \bar{\omega}, \tag{4.3}$$

where the pull-back of $\bar{\omega}$ is

$$\phi_t^* \bar{\omega}\big|_{\boldsymbol{x}} = \big(\phi_t^* \bar{\sigma}(\boldsymbol{x})\big) \phi_t^* \omega\big|_{\boldsymbol{x}} \tag{4.4a}$$

$$= \frac{\bar{\sigma}(\phi_t \boldsymbol{x})}{\bar{\sigma}(\boldsymbol{x})} \exp\left[\int_0^t \mathrm{d}s\, \kappa(\phi_s \boldsymbol{x})\right] \bar{\omega}\bigg|_{\boldsymbol{x}}. \tag{4.4b}$$

For $\bar{\omega}$ absolutely continuous with respect to ω, the invariance property

$$\phi_t^* \bar{\omega} = \bar{\omega} \tag{4.5}$$

holds for all $\boldsymbol{x}$ except possibly a set of ω-measure zero [60,61]; that is,

$$\bar{\sigma}(\phi_t \boldsymbol{x}) = \bar{\sigma}(\boldsymbol{x}) \exp\left[-\int_0^t \mathrm{d}s\, \kappa(\phi_s \boldsymbol{x})\right] \tag{4.6}$$

almost everywhere.

Setting

$$\bar{\sigma}(\boldsymbol{x}) \equiv \mathrm{e}^{-w(\boldsymbol{x})}, \tag{4.7}$$

relation (4.6) will hold provided the compressibility κ is the derivative of the *time-independent* function $w(\boldsymbol{x})$ along the flow $\boldsymbol{\xi}$

$$\kappa = \xi^i_{,i} = \mathcal{L}w = \xi^i \frac{\partial w}{\partial x^i}, \tag{4.8}$$

in which case

$$\exp\left[\int_0^t \mathrm{d}s\,\kappa(\phi_s \boldsymbol{x})\right] = \exp\left[w(\phi_t \boldsymbol{x}) - w(\boldsymbol{x})\right] \tag{4.9}$$

and

$$\bar{\sigma}(\phi_t \boldsymbol{x}) = \bar{\sigma}(\boldsymbol{x})\mathrm{e}^{-[w(\phi_t \boldsymbol{x}) - w(\boldsymbol{x})]} \tag{4.10}$$

for *all* $\boldsymbol{x}$.

For the non-Hamiltonian systems that have been used to simulate various equilibrium ensembles, it is possible to write the compressibility as the Lie derivative of a well-behaved function (see [37]). The choice of volume form $\bar{\omega} = \mathrm{e}^{-w(\boldsymbol{x})}\omega$ therefore renders the dynamics incompressible; such a system satisfies the condition for Poincaré recurrences (for compact phase space) [62], and, provided the actual dynamics is ergodic, equilibrium averages with respect to $\bar{\omega}$ can be obtained by computing time averages over single trajectories.

A familiar example is the equilibrium Nosé–Hoover system [63], $\boldsymbol{x} = (q, p, p_\eta)$,

$$\dot{q} = \frac{p}{m}, \tag{4.11a}$$

$$\dot{p} = F(q) - \alpha p p_\eta, \tag{4.11b}$$

$$\dot{p}_\eta = \left[\frac{p^2}{m} - kT\right], \tag{4.11c}$$

where $\Phi(q)$ is the system potential energy, $F(q) = -\partial\Phi(q)/\partial q$, α is a coupling parameter, k is Boltzmann's constant and T the temperature of the thermostat. The phase space compressibility is

$$\kappa(q, p, p_\eta) = \frac{\partial \dot{q}}{\partial q} + \frac{\partial \dot{p}}{\partial p} + \frac{\partial \dot{p}_\eta}{\partial p_\eta} = -\alpha p_\eta. \tag{4.12}$$

Setting

$$w(q, p, p_\eta) = \frac{1}{kT}\left\{\frac{p^2}{2m} + \Phi(q) + \alpha\frac{p_\eta^2}{2}\right\} \tag{4.13}$$

we find

$$\mathcal{L}\, w = \left[\dot{q}\frac{\partial}{\partial q} + \dot{p}\frac{\partial}{\partial p} + \dot{p}_\eta\frac{\partial}{\partial p_\eta}\right] w = -\alpha p_\eta = \kappa, \tag{4.14}$$

so that

$$\bar{\omega} = \exp\left[-\frac{1}{kT}\left\{\frac{p^2}{2m} + \Phi(q) + \alpha\frac{p_\eta^2}{2}\right\}\right] \mathrm{d}q \wedge \mathrm{d}p \wedge \mathrm{d}p_\eta \tag{4.15}$$

is an invariant volume form [63]. (For a 1D harmonic oscillator coupled to a thermostat, the flow (4.11) is not ergodic [64], implying the existence of additional dynamical constraints [37].)

For a general non-Hamiltonian system, consider a phase point $\boldsymbol{x}$ that lies on a periodic orbit of period T, so that $\phi_T \boldsymbol{x} = \boldsymbol{x}$. As $\boldsymbol{x}$ and $\phi_T \boldsymbol{x}$ are the same phase point, the density $\bar{\sigma}$ must satisfy

$$\bar{\sigma}(\phi_T \boldsymbol{x}) = \bar{\sigma}(\boldsymbol{x}). \tag{4.16}$$

This condition is consistent with (4.10) for $\boldsymbol{x} = \phi_T \boldsymbol{x}$. If, however, the periodic orbit is *net* contracting or expanding, so that

$$\exp\left[\int_0^T \mathrm{d}s\, \kappa(\phi_s \boldsymbol{x})\right] \neq 1, \tag{4.17}$$

where the integral is evaluated along the periodic orbit, conditions (4.6) ($t = T$) and (4.16) cannot be satisfied simultaneously for points on the periodic orbit. (Such periodic orbits cannot exist in a Hamiltonian system.)

We have therefore shown that the presence of *net* attracting or repelling periodic orbits or fixed points precludes the existence of a smooth invariant measure. This is a basic theorem of ergodic theory (see [47, chapter 2, section 1]). In such a case we must conclude either that it is not possible to write κ in the form (4.8), or that the function $w(\boldsymbol{x})$ is not well-behaved (singular).

The assumption of a smooth invariant measure [35–37] cannot therefore be generally valid for non-Hamiltonian systems. Conversely, all periodic orbits in systems for which it possible to find a smooth stationary volume element must have stability matrices with unit determinant.

The essential difference between a system for which the compressibility can be written as $\kappa = \mathcal{L}w$ and one for which this relation does not hold is nicely illustrated by the example of the Nosé–Hoover system generalized to have a coordinate-dependent temperature, $T(q)$ [65]. The dynamical equations, which model a system subject to a temperature gradient, are by no means unique. One approach is to generalize the standard Nosé Hamiltonian treatment (cf. the appendix of [65]). For a system with a single degree of freedom (q, p) and thermostat variables (η, p_η), this procedure yields the equations of motion

$$\dot{q} = \frac{p}{m}, \tag{4.18a}$$

$$\dot{p} = F(q) - \alpha p p_\eta - \eta k T'(q), \tag{4.18b}$$

$$\dot{\eta} = \alpha p_\eta, \tag{4.18c}$$

$$\dot{p}_\eta = \left[\frac{p^2}{m} - kT(q)\right], \tag{4.18d}$$

where $T' \equiv \mathrm{d}T/\mathrm{d}q$. Although, as a result of a non-canonical change of variables and a time-scaling, the equations (4.18) are not in Hamiltonian form, the Hamiltonian function

$$H_N = \frac{p^2}{2m} + \Phi(q) + \frac{\alpha p_\eta^2}{2} + \eta k T(q) \tag{4.19}$$

is nevertheless a constant of the motion. For fixed $H_N = E_N$ we therefore have the relation

$$\eta = \eta(p, q, p_\eta; E_N), \tag{4.20}$$

so that the reduced flow $\boldsymbol{\xi} \equiv (\dot{q}, \dot{p}, \dot{p}_\eta)$ on the E_N-shell is given by (cf. equation (4.11))

$$\dot{q} = \frac{p}{m}, \tag{4.21a}$$

$$\dot{p} = F(q) - \alpha p p_\eta - \frac{T'}{T}\left[E_N - \frac{p^2}{2m} - \Phi(q) - \alpha\frac{p_\eta^2}{2}\right], \tag{4.21b}$$

$$\dot{p}_\eta = \left[\frac{p^2}{m} - kT(q)\right]. \tag{4.21c}$$

The compressibility is

$$\kappa = \mathrm{div}_\omega(\boldsymbol{\xi}) = \frac{\partial\dot{q}}{\partial q} + \frac{\partial\dot{p}}{\partial p} + \frac{\partial\dot{p}_\eta}{\partial p_\eta} = -\alpha p_\eta + \frac{p}{m}\frac{T'}{T}, \tag{4.22}$$

and can be written as the Lie derivative of the function $w(p, q, p_\eta; E_N)$, where

$$w(p, q, p_\eta; E_N) \equiv \ln\bigl(kT(q)\bigr) - \frac{1}{kT(q)}\left\{E_N - \frac{p^2}{2m} - \Phi(q) - \frac{\alpha p_\eta^2}{2}\right\}. \tag{4.23}$$

The function

$$\bar{\sigma}(p, q, p_\eta; E_N) \equiv \frac{1}{kT(q)}\exp\left[\frac{1}{kT(q)}\left\{E_N - \frac{p^2}{2m} - \Phi(q) - \frac{\alpha p_\eta^2}{2}\right\}\right] \tag{4.24}$$

is therefore a stationary solution of the GLE, yielding an invariant volume form $\bar{\omega}$. In the limit that T is independent of q, the invariant distribution (4.24) reduces to the solution obtained above for the simple Nosé–Hoover system.

On the other hand, following Posch and Hoover [65], one can simply postulate the dynamical equations

$$\dot{q} = \frac{p}{m}, \tag{4.25a}$$

$$\dot{p} = F(q) - \alpha p p_\eta, \tag{4.25b}$$

$$\dot{p}_\eta = \left[\frac{p^2}{m} - kT(q)\right], \tag{4.25c}$$

which are perhaps the simplest possible generalization of the constant T equations (4.11). This system has been studied numerically and appears to exhibit a fractal nonequilibrium steady state [65]. The existence of attracting periodic orbits has moreover been established numerically, thus precluding the existence of any smooth invariant measure [65].

There is therefore a fundamental qualitative difference between the dynamical system (4.21), which has a smooth invariant volume form and incompressible dynamics, and the dissipative system (4.25), for which it is impossible to write κ as $\mathcal{L}w$, and which exhibits attracting periodic orbits and fractal phase space structure.

The possibility of a singular invariant density is exemplified by the very simple system

$$\dot{x} = -\alpha x, \tag{4.26a}$$

$$\dot{y} = +\beta y, \tag{4.26b}$$

with real parameters $\alpha, \beta > 0$, and $\alpha > \beta$, so that the fixed point $(0, 0)$ is net attractive. In this case, the compressibility is constant,

$$\kappa = -(\alpha - \beta), \tag{4.27}$$

and can be written as

$$\kappa = \mathcal{L}\big(\ln|x| + \ln|y|\big). \tag{4.28}$$

The invariant density is therefore

$$\bar{\sigma} = \frac{1}{|x||y|}, \tag{4.29}$$

which is singular both at the origin and along the stable and unstable manifolds of the fixed point (x-axis and y-axis, respectively). The resulting invariant measure $\bar{\omega}$ is not absolutely continuous with respect to $\omega = \mathrm{d}x \wedge \mathrm{d}y$.

To summarize: the standard definition of an invariant volume form $\bar{\omega}$ requires that the function $\bar{\sigma}$ be a stationary solution of the GLE [22,47]. The existence of attracting or repelling periodic orbits precludes the existence of a smooth invariant measure.

A generalization of the notion of invariant volume form to include the possibility of time-dependent functions $\bar{\sigma}$ has been proposed [37]. This possibility is discussed in the next subsection.

4.2. Time-dependent volume forms satisfying the transport equation

We now generalize the preceding discussion and allow the density $\bar{\sigma}_t \equiv \bar{\sigma}(t, \boldsymbol{x})$ to depend explicitly on time. Suppose also that it satisfies the GLE (3.16), so that $\bar{\omega}_t$ satisfies the transport equation (3.5), $\phi_t^* \bar{\omega}_t = \bar{\omega}_0$. For any region $\mathcal{R}$ we therefore have conservation of ensemble members (cf. equation (3.3b))

$$\int_{\phi_t \mathcal{R}} \bar{\omega}_t = \int_{\mathcal{R}} \phi_t^* \bar{\omega}_t = \int_{\mathcal{R}} \bar{\omega}_0. \tag{4.30}$$

Equations (4.1) and (4.30) are superficially similar; only in equation (4.1), however, is an invariant measure actually defined. TEA have nevertheless proposed that time-dependent forms such as $\bar{\omega}_t$ be considered as generalized invariant volume elements [37]. The function $\bar{\sigma}$ (denoted $\sqrt{g}$ by TEA [37], see section 6) is to be computed by the method of characteristics; that is, the initial condition $\bar{\sigma}(t = 0, \boldsymbol{x})$ is specified for all $\boldsymbol{x}$, and $\bar{\sigma}(t, \phi_t \boldsymbol{x})$ obtained by integration along trajectories:

$$\frac{\mathrm{d}\bar{\sigma}}{\mathrm{d}t} = \frac{\partial \bar{\sigma}}{\partial t} + \mathcal{L}\bar{\sigma} = -\kappa\bar{\sigma}. \tag{4.31}$$

There are several points to be made concerning this proposal. We note again that a time-dependent form $\bar{\omega}_t$ cannot be an invariant volume form according to the standard mathematical definition [47]. Such a time-dependent volume form would result in the "size" of a fixed region of phase space fluctuating with time [46]. As long as the vector field $\boldsymbol{\xi}$ is time-independent, the volume form $\bar{\omega}_t$ *is*, however, an invariant n-form in $(n + 1)$-dimensional *extended phase space* (phase space augmented to include the time t as a coordinate); that is,

$$\mathcal{L}'\bar{\omega}_t = 0, \tag{4.32}$$

where $\mathcal{L}'$ is the Lie derivative associated with the extended vector field [15,18,48]

$$\boldsymbol{\xi}' = \boldsymbol{\xi} + \frac{\partial}{\partial t}. \tag{4.33}$$

Although the function $\bar{\sigma}(t, \boldsymbol{x})$ is single-valued in extended phase space, it is not necessarily single-valued in $\boldsymbol{x}$-space; consider the example of a phase point on a net attracting/repelling periodic orbit, for which the value of $\bar{\sigma}$ decreases/increases after each traversal of the orbit.

To define a true invariant density, one should consider the limiting ($t \to \infty$) behavior of the density n-form ρ_t [32]. Although a time-dependent solution of the transport equation ρ_t does not define an invariant density, either the infinite-time limit or the infinite-time average of ρ_t,

$$\mu_\infty = \lim_{T\to\infty} \int_0^T \mathrm{d}t\, \rho_t, \tag{4.34}$$

can be used to define an invariant measure [32]. If ρ is chosen to be absolutely continuous with respect to ω at $t = 0$, then ρ_t remains absolutely continuous for all finite t [32]. However, the infinite-time average invariant measure (assumed to exist) describing the nonequilibrium steady state is for many systems a measure such as the SRB measure [26], which is "singular" (that is, not absolutely continuous with respect to ω). The SRB measure and related "fractal" measures are relevant objects of study for nonequilibrium steady states [26,32,59]. Although for finite times a time-dependent solution $\bar{\sigma}$ of the GLE with smooth initial condition cannot exhibit the singular structure of the true invariant measure in the nonequilibrium steady state, at long times $\bar{\sigma}$ will presumably become more and more convoluted and more nearly singular as it attempts to mimic the fractal invariant measure. In this sense, direct numerical solution of the GLE to describe the nonequilibrium steady state becomes less and less useful at long times [34,46]. Formally, the infinite-time average of a phase function $\langle B\rangle(t)$ is then equivalent to an average over the invariant measure μ_∞ (4.34).

5. Time-evolution of the Gibbs entropy

5.1. Definition and properties of entropy

The Gibbs entropy $S_{\bar{\omega}}$ associated with the volume form $\bar{\omega}$ is defined as the information entropy of the distribution function $\bar{f}$ with respect to $\bar{\omega}$

$$S_{\bar{\omega}} \equiv -\int_{\mathcal{M}} (\bar{f} \ln \bar{f})\bar{\omega} = -\int_{\mathcal{M}} (\ln \bar{f})\rho, \tag{5.1}$$

where $\rho = \bar{f}\bar{\omega}$. The expression for $S_{\bar{\omega}}$ is manifestly coordinate-independent for a particular choice of the n-form $\bar{\omega}$, but its value clearly depends on the choice of $\bar{\omega}$. For the moment, we allow the volume form $\bar{\omega}$ to be time-dependent.

The time derivative of $S_{\bar{\omega}}$ is

$$\frac{\mathrm{d}S_{\bar{\omega}}}{\mathrm{d}t} = -\int_{\mathcal{M}} \{\partial_t \bar{f}[1 + \ln \bar{f}]\bar{\omega} + (\bar{f} \ln \bar{f})\partial_t \bar{\omega}\}. \tag{5.2}$$

Use of the general transport equation (3.13) allows us to write the time derivative as

$$\frac{\mathrm{d}S_{\bar{\omega}}}{\mathrm{d}t} = \int_{\mathcal{M}} \{[1 + \ln \bar{f}]((\mathcal{L}\bar{f})\bar{\omega} + \bar{f}(\mathcal{L}\bar{\omega})) + \bar{f}\partial_t \bar{\omega}\}. \tag{5.3}$$

Integration by parts, or equivalently application of Stokes' theorem (assuming boundary terms vanish) yields the general expression for the time derivative of $S_{\bar{\omega}}$:

$$\frac{\mathrm{d}S_{\bar{\omega}}}{\mathrm{d}t} = \int_{\mathcal{M}} \bar{f}[\partial_t \bar{\omega} + \mathcal{L}\bar{\omega}]. \tag{5.4}$$

As in the discussion of the transport equation, several special cases are possible. First, suppose that the volume form $\bar{\omega}$ is time-independent, $\partial_t \bar{\omega} = 0$. From (5.4) we have

$$\frac{\mathrm{d}S_{\bar{\omega}}}{\mathrm{d}t} = \int_{\mathcal{M}} \bar{f}(\mathcal{L}\bar{\omega}) = \int_{\mathcal{M}} (\mathrm{div}_{\bar{\omega}}\boldsymbol{\xi})\rho. \tag{5.5}$$

This is the well-known result that the time derivative of $S_{\bar{\omega}}$ is equal to the phase space average of the $\bar{\omega}$-divergence of the vector field $\boldsymbol{\xi}$ [13–22].

If the n-form $\bar{\omega}$ is time-dependent, but itself satisfies the transport equation (3.7), then the time-derivative of $S_{\bar{\omega}}$ is zero, as anticipated from the incompressible time evolution (3.17). This is the case considered in [37].

If $\bar{\omega}$ is both time-independent *and* invariant, $\mathcal{L}\bar{\omega} = 0$, the time-derivative of the entropy vanishes

$$\frac{\mathrm{d}S_{\bar{\omega}}}{\mathrm{d}t} = 0. \tag{5.6}$$

This is the case for the usual entropy S_{ω} defined for Hamiltonian systems, where the standard volume form ω is invariant (Liouville's theorem). In general, if a stationary volume form $\bar{\omega}$ can be found such that the vector field $\boldsymbol{\xi}$ is divergenceless, $\mathrm{div}_{\bar{\omega}}\boldsymbol{\xi} = 0$, then the associated entropy $S_{\bar{\omega}}$ is constant.

5.2. Coordinate independence of entropy and dependence on volume form

In their discussion of the properties of the generalized Gibbs entropy for non-Hamiltonian systems, TEA have stressed the apparent "coordinate dependence" of earlier formulations [37].

There are really two relevant notions of coordinate dependence here. The first concerns the invariance of expressions for the generalized Gibbs entropy under transformations of coordinate system. As we have stressed above, any quantity written in terms of forms is by definition invariant under changes of coordinate system [6–8]. The second concerns the dependence of the entropy $S_{\bar{\omega}}$ on the choice of volume form $\bar{\omega}$. Only by changing the volume form from $\bar{\omega}$ to $\bar{\omega}'$, say, can we change the value of $\dot{S}$. Again, the value of $\dot{S}$ will be the same in any coordinate system when using the volume form $\bar{\omega}'$.

By requiring the (in general) time-dependent n-form $\bar{\omega}_t$ to satisfy the transport equation (3.7), a constant value of the entropy is obtained, independent of the coordinate system $\boldsymbol{x}$ used to define the decomposition of the volume form $\bar{\omega}$:

$$\bar{\omega} = \bar{\sigma}_{\boldsymbol{x}} \omega_{\boldsymbol{x}}. \tag{5.7}$$

If $\bar{\omega}$ is time-independent, then the choice of the stationary invariant volume form $\bar{\omega}$ renders the flow incompressible, $\mathrm{div}_{\bar{\omega}} \boldsymbol{\xi} = 0$ [22]. If, on the other hand, it is necessary for the volume form $\bar{\omega}_t$ to depend explicitly on time in order to ensure that $\dot{S}_{\bar{\omega}_t} = 0$, then the constancy of $S_{\bar{\omega}_t}$, although formally correct, is devoid of fundamental physical significance. This is because all the "interesting" compressible dynamics is reflected in the (metric) factor $\bar{\sigma}$, which is a nonstationary solution of the GLE (see below).

6. Invariant volume forms and compatible metric tensors

6.1. Time-independent metric

Our treatment of non-Hamiltonian systems up to this point makes no use of any Riemannian structure of phase space. In fact, all the results obtained do not in any way require the existence of a metric tensor in phase space (see also the discussion in [51]).

In order to make closer contact with the work of TEA, however, we now assume the existence of a metric tensor $\boldsymbol{g}$ on the phase space manifold $\mathcal{M}$ [35–37]. We therefore define a metric (symmetric) tensor field $\boldsymbol{g}(\boldsymbol{x})$

$$\boldsymbol{g}(\boldsymbol{x}) = g(\boldsymbol{x})_{ij}\, \mathrm{d}x^i \otimes \mathrm{d}x^j, \tag{6.1}$$

where the tensor elements g_{ij} are assumed to be single-valued, continuous, continuously differentiable, etc. We also assume for the moment that the tensor $\boldsymbol{g}$ does not depend explicitly on time (this follows [35,36]; the time-dependent case [37] is considered below). Associated with the metric tensor is the standard Riemannian volume form [7,8]

$$\sqrt{g}(\boldsymbol{x})\omega = \sqrt{g}(\boldsymbol{x})\, \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \cdots \wedge \mathrm{d}x^n, \tag{6.2}$$

where g is the determinant of the metric tensor g_{ij}.

The metric tensor $\boldsymbol{g}$ enables the inner product of two tangent vectors to be defined: for $\boldsymbol{u}, \boldsymbol{v} \in T_{\boldsymbol{x}}\mathcal{M}$, the inner product is

$$\boldsymbol{u} \cdot \boldsymbol{v}\big|_{\boldsymbol{x}} \equiv g(\boldsymbol{x})_{ij} u^i v^j. \tag{6.3}$$

For the metric tensor to be *compatible* with the flow induced by the vector field $\boldsymbol{\xi}$ [6], ϕ_t must be an *isometry* for all t. That is, the inner product of two tangent vectors must be preserved under the flow ϕ_t:

$$\boldsymbol{u} \cdot \boldsymbol{v}\big|_{\boldsymbol{x}} = \phi_{t*}\boldsymbol{u} \cdot \phi_{t*}\boldsymbol{v}\big|_{\phi_t \boldsymbol{x}}, \tag{6.4}$$

where ϕ_{t*} is the derivative mapping, and $\phi_{t*}\boldsymbol{u}, \phi_{t*}\boldsymbol{v} \in T_{\phi_t \boldsymbol{x}}\mathcal{M}$. Condition (6.4) will not be satisfied for arbitrary metric tensor fields $\boldsymbol{g}$. In terms of components, (6.4) implies that

$$g(\boldsymbol{x})_{i'j'} = \frac{\partial(\phi_t x)^i}{\partial x^{i'}} g(\phi_t \boldsymbol{x})_{ij} \frac{\partial(\phi_t x)^j}{\partial x^{j'}}. \tag{6.5}$$

The compatibility condition between the metric tensor $\boldsymbol{g}$ and the flow $\boldsymbol{\xi}$ is equivalent to the requirement that $\boldsymbol{\xi}$ be a Killing vector for $\boldsymbol{g}$ [6]; in terms of the Lie derivative,

$$\mathcal{L}\boldsymbol{g} = 0, \tag{6.6a}$$

or, in component form [6–8],

$$g_{ij,k}\xi^k + g_{kj}\xi^k_{,i} + g_{ik}\xi^k_{,j} = 0. \tag{6.6b}$$

Using the symmetry of the metric tensor, $g_{ij} = g_{ji}$, and multiplying by the inverse matrix g^{ij} yields

$$g^{ij} g_{ij,k}\xi^k = -2\xi^k_{,k}. \tag{6.7}$$

We have

$$g^{ij} g_{ij,k} = 2\Gamma^j_{jk}, \tag{6.8}$$

and

$$\Gamma^j_{jk} = \frac{1}{\sqrt{g}} \frac{\partial \sqrt{g}}{\partial x^k} = \frac{\partial \ln \sqrt{g}}{\partial x^k}, \tag{6.9}$$

where Γ^i_{jk} is the usual metric connection [6,8],

$$\Gamma^i_{jk} \equiv \frac{1}{2} g^{ii'}[g_{i'j,k} + g_{i'k,j} - g_{jk,i'}]. \tag{6.10}$$

The compatibility condition therefore requires that the phase space compressibility be given by the expression

$$\kappa = \xi^k_{,k} = -\xi^k \frac{\partial \ln \sqrt{g}}{\partial x^k} = -\mathcal{L} \ln(\sqrt{g}), \tag{6.11}$$

which is precisely of the form (4.8). That is, the function $\sqrt{g} = \mathrm{e}^{\ln(\sqrt{g})}$ is a stationary solution of the GLE,

$$\mathrm{div}_{\omega}\big(\sqrt{g}\boldsymbol{\xi}\big) = \frac{\partial}{\partial x^k}\big[\mathrm{e}^{\ln(\sqrt{g})}\xi^k\big] = 0, \tag{6.12}$$

and the volume form

$$\bar{\omega} = \sqrt{g}\omega \tag{6.13}$$

is invariant under the flow.

6.2. Time-dependent metric

As discussed in section 4, for general non-Hamiltonian systems it is not possible to write the compressibility as the directional derivative of a smooth, time-independent function, so that a smooth time-independent metric tensor compatible with the flow does not exist. Following [37], however, we can generalize the above discussion of the stationary metric by considering a time-dependent metric tensor.

It should immediately be recognized that, by suitable choice of a time-dependent metric, *any* local dynamical behavior whatsoever can be imposed upon the system (for example, rate of divergence of nearby trajectories) [49,50]. The definition of the time-dependent metric tensor used in [37] is then precisely that required to "undo" the natural contraction/expansion of the comoving volume element [41].

Defining the time-dependent metric tensor field $\boldsymbol{g}(t, \boldsymbol{x})$

$$\boldsymbol{g}(t, \boldsymbol{x}) = g(t, \boldsymbol{x})_{ij}\, \mathrm{d}x^i \otimes \mathrm{d}x^j, \tag{6.14}$$

the tensor elements g_{ij} are now explicit functions of time, and the associated Riemannian volume form is

$$\bar{\omega}_t = \sqrt{g}(t, \boldsymbol{x})\omega. \tag{6.15}$$

The suitably generalized invariance condition is

$$\boldsymbol{u} \cdot \boldsymbol{v}\big|_{t=0,\boldsymbol{x}} = \phi_{t*}\boldsymbol{u} \cdot \phi_{t*}\boldsymbol{v}\big|_{t,\phi_t\boldsymbol{x}}, \tag{6.16}$$

or, in terms of components,

$$g(0, \boldsymbol{x})_{i'j'} = \frac{\partial(\phi_t x)^i}{\partial x^{i'}} g(t, \phi_t\boldsymbol{x})_{ij} \frac{\partial(\phi_t x)^j}{\partial x^{j'}}. \tag{6.17}$$

Equation (6.16) is an invariance condition in extended phase space, $(t, \boldsymbol{x})$, *not* in ordinary phase space $\boldsymbol{x}$. In terms of the Lie derivative, the compatibility condition on $\boldsymbol{g}$ is

$$\frac{\partial \boldsymbol{g}}{\partial t} + \mathcal{L}_{\boldsymbol{\xi}}\boldsymbol{g} = 0, \tag{6.18a}$$

or, in component form,

$$\frac{\partial g_{ij}}{\partial t} + g_{ij,k}\xi^k + g_{kj}\xi^k_{,i} + g_{ik}\xi^k_{,j} = 0. \tag{6.18b}$$

Following the argument of the previous subsection, we see that the function $\sqrt{g}(t, \boldsymbol{x})$ must satisfy the equation

$$\frac{\mathrm{d}\sqrt{g}}{\mathrm{d}t} = \frac{\partial\sqrt{g}}{\partial t} + \mathcal{L}\sqrt{g} = -\kappa\sqrt{g}. \tag{6.19}$$

That is, $\sqrt{g}$ *is itself a time-dependent solution of the GLE* (3.10), and the associated Riemannian volume form $\bar{\omega}_t = \sqrt{g}\omega$ satisfies the transport equation,

$$\frac{\partial\bar{\omega}_t}{\partial t} + \mathcal{L}\bar{\omega}_t = 0. \tag{6.20}$$

As we have emphasized above, introduction of a time-dependent metric tensor does not in any way solve the problem of determining an invariant probability density for general non-Hamiltonian systems. The fact that $\sqrt{g}$ must satisfy the GLE in order for the metric tensor to be compatible with the flow implies that the associated density $\bar{f}$ will be a solution of the Liouville equation for incompressible flow, and the entropy $S_{\bar{\omega}}$ will be constant. This simply means that, in solving the GLE by first obtaining $\sqrt{g}$, and then finding the density $\bar{f}$ whose evolution is governed by incompressible flow, we have placed all the burden of describing the compressible dynamics on the metric factor $\sqrt{g}$ (cf. also [46]). The need to solve the original GLE with compressible dynamics of course remains, as we must determine $\sqrt{g}$ itself!

There is a considerable degree of arbitrariness in the determination of the metric tensor $\boldsymbol{g}(t, \boldsymbol{x})$ and the function $\sqrt{g}$. In solution of the generalized GLE by the method of characteristics, the initial metric factor $\sqrt{g}(t = 0, \boldsymbol{x})$ is essentially arbitrary, so that, in cases where there is no stationary metric compatible with the flow, the phase space "geometry" determined by $\sqrt{g}$ is by no means unique. (Lyapunov exponents determined by infinite time average contraction/expansion rates are, however, unique [31,66].)

As it is in general necessary to solve the full compressible GLE to obtain the time-dependent metric factor $\sqrt{g}$, the resulting constancy of the entropy $S_{\bar{\omega}}[\bar{f}]$ associated with the introduction of trajectory-dependent expansion/contraction factors [37] is of purely formal significance. The metric factor cannot in general be written explicitly as a function of the instantaneous phase point only, and each trajectory must effectively be endowed with a "demon" who follows the phase point and diligently undoes the natural contraction/expansion associated with the actual compressible dynamics.

7. Summary and conclusion

In this paper we have discussed several fundamental questions concerning the statistical mechanics of non-Hamiltonian systems. Following Steeb [18], we have applied the theory of differential forms to obtain a fully covariant formulation of the generalized Liouville equation governing the dynamics of the phase space distribution function. By basing our approach on the density n-form, and the associated transport/continuity equation, we obtain a formulation that is not only manifestly coordinate-independent, but also independent of the choice of volume form on the phase space manifold.

The properties of invariant volume forms are of great importance in the theory of non-Hamiltonian systems. In particular, there has been considerable recent interest in the question of smoothness versus fractality of the invariant measure [35,36,41,44,45]. Our discussion of the properties of invariant volume forms has emphasized the fact that invariant densities are by definition stationary solutions of the GLE [22,47,60]. We also point out that the existence of net attractive or repulsive periodic orbits precludes the existence of a smooth invariant measure [47]. While time-dependent solutions of the Liouville equation do not define invariant densities, an invariant measure can be obtained by taking the infinite-time average of the time-dependent density n-form [32].

We have examined the properties of the Gibbs entropy associated with a given volume form. Although the expression for the entropy is manifestly coordinate-independent, the value of the entropy clearly depends on the particular volume form chosen. We have examined the time evolution of the entropy, and have noted that the choice of a time-dependent volume form satisfying the transport equation leads to a constant value of the entropy, so that the associated distribution function obeys an evolution equation associated with incompressible flow [7,37,48]. For general non-Hamiltonian systems this result [37] is of purely formal significance, as all the “interesting” non-Hamiltonian dynamics are in fact reflected in the time-evolution of the volume form itself (see also the discussion of this point in [46]).

Our formulation of non-Hamiltonian dynamics does not depend in any way on the phase space manifold possessing any Riemannian structure (metric tensor). For non-Hamiltonian flows on a manifold with metric, we show that compatibility of the metric tensor with the flow (that is, the requirement that the flow be an isometry) implies that the metric factor must be a solution of the GLE. This metric factor is in general time-dependent, and so does not define an invariant measure in the conventional sense. Relevant solutions of the GLE are by no means unique, and hence the “geometry” of the manifold is not uniquely defined.

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