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Entropy production and phase space volume contraction

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We inquire whether the connection between entropy production and phase space volume contraction rate reported recently for a class of thermostatted systems is an intrinsic property of a wide class of dynamical systems, or the result of the particular algorithm devised for thermostatting a system of interacting particles obeying, in the presence of nonequilibrium constraints, a time-reversible, dissipative dynamics. A nonequilibrium thermodynamics based on the balance equation for information entropy is developed for dissipative dynamical systems subjected, in addition, to a stochastic forcing. This latter accounts for the thermodynamic fluctuations accompanying the reduced description of the thermostat by a dissipative perturbation, for the interaction between the system and the external reservoirs or for perturbations of external origin. Entropy flux and entropy productionlike terms depending on the characteristics of the dynamics in phase space, particularly the rate of phase space volume contraction, are identified. Their connections with irreversible thermodynamics are explored. In particular, for thermostatted systems we find, without invoking an *ad hoc* conservation law between the system and the reservoir, that information entropy production is related to the opposite of the rate of phase space volume contraction to the second order in the distance from equilibrium.

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I. INTRODUCTION

Recently, a number of relationships linking phase space dynamics to thermodynamic quantities like entropy production and Onsager coefficients have been put forward [1–7]. In their general setting they are concerned with an initially isolated conservative system subjected subsequently to a dissipative perturbation, describing the combined effect of an external constraint and of a thermostat. As such a system possesses an (generally multifractal) attractor, it will undergo on average a contraction of the phase space volume,

$$\lim_{t\to\infty} \overline{\frac{d}{dt}\ln \Delta\Gamma(t)^t} = \sum_i \sigma_i < 0 \tag{1}$$

where σ_i are the (mean) Lyapunov exponents [8]. The rate of this contraction $|\overline{d\ln\Delta\Gamma(t)/dt^t}|$ is then *defined* by some authors as the entropy production of the dynamical system on the grounds of its positivity [5,7]. Alternatively, in certain types of thermostatted Hamiltonian systems it is shown to be equal in the nonequilibrium steady state to the work per unit time performed on the system by the external constraints, which is in turn formally proportional to the expression of intrinsic entropy production as given by irreversible thermodynamics.

As is well known, phase space contraction is also given by the time derivative of the Gibbs entropy,

$$S_G = -\int d\mathbf{x}\,\rho(\mathbf{x},t)\ln\rho(\mathbf{x},t), \tag{2}$$

where $\mathbf{x}=\{x_i\}$ denotes the set of phase space coordinates, provided that the rate of change of the probability density ρ is evaluated from the Liouville equation

$$\lim_{t\to\infty}\frac{dS_G}{dt} = \sum_i \sigma_i < 0. \tag{3}$$

One is then led immediately to the paradoxical conclusion that in such systems Gibbs entropy decreases without limit for long times and becomes eventually unbounded, thereby precluding the existence of a steady state value $\lim_{t\to\infty} S_G = -\infty$. This is to be related to the singularity of the invariant density ρ_s, confined on an object—the attractor—whose information dimension is strictly less than that of the embedding phase space.

Inasmuch as irreversible thermodynamics, in particular the distinction between entropy flux and entropy production, must be generated from a balance equation describing how entropy evolves in time within the system, the result summarized in Eq. (3) seems to preclude the possibility of building a self-consistent thermodynamics of the above defined thermostatted systems. It is indeed not clear why one can plainly use the expression of entropy production of classical irreversible thermodynamics, which finds its origin in quite different assumptions such as local equilibrium and the Gibbs entropy postulate. One is thus led to inquire whether the connection between entropy production and phase space volume contraction (or equivalently Lyapunov exponents) stipulated in recent literature is an intrinsic property, a matter of definition, or the result of the particular algorithm devised for thermostatting the system. One might even argue that under the setting of Eqs. (1)–(3) there is no place for entropy production at all: as the system collapses toward the attractor, it merely experiences an (negative) entropy flux, reflecting the fact that time going on its localization in phase space becomes increasingly sharper.

The difficulties summarized above are sufficiently compelling to warrant an alternative approach and a complemen-

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tary viewpoint. Our objective in the present work is to outline a step in this direction accounting for the following features: To identify a general class of dynamical systems for which a link between phase space dynamics and thermodynamiclike quantities may be established; to generate for such systems, in a self-consistent manner, a thermodynamic formalism bearing a direct link with the entropy production of classical irreversible thermodynamics; and to provide an alternative approach to thermostatted systems in the light of this formalism, free of the singularities of the entropy pointed out in connection with Eq. (3).

The general formulation, based on the introduction of fluctuating forces along with the action of the dissipative perturbation, is laid down in Sec. II. In Sec. III a balance equation for the information entropy is derived, from which two alternative forms of (information) entropy production are identified. A more explicit form of these terms is derived in Secs. IV and V for the particular classes of thermostatted and mesoscopic systems, respectively, leading to an explicit relation with thermodynamic entropy production. The main conclusions are drawn in Sec. VI.

II. GENERAL FORMULATION

In what follows we shall be concerned with systems whose state vector $\mathbf{x}=(x_1,\ldots,x_n)$ satisfies the following generic form of evolution equations:

$$\frac{d\mathbf{x}}{dt}=\mathbf{F}(\mathbf{x},\mu)+\mathbf{R}(t). \tag{4}$$

The evolution operator $\mathbf{F}$, the control parameter μ and the stochastic forcing $\mathbf{R}$ are designed to account for the following situations:

(i) The evolution operator $\mathbf{F}$ is a dissipative operator, in the sense of

$$\overline{\operatorname{div}\mathbf{F}}^{t}<0, \quad t\geqslant t_0. \tag{5}$$

It may describe the evolution of a set of macroscopic observables, or the evolution of microscopic degrees of freedom of an initially conservative system put subsequently in contact with a thermostat and subjected to a dissipative perturbation removing it from equilibrium.

(ii) The control parameter μ monitors the thermodynamic behavior of the system,

$$\mu=\mu_e+h, \tag{6}$$

μ_e being the equilibrium value and h the deviation from equilibrium. We emphasize that in this formulation the evolution operator $\mathbf{F}$ remains dissipative in equilibrium. (Canonical) equilibrium is nevertheless achieved, provided that the forcing term $\mathbf{R}$ satisfies certain conditions, as discussed further below.

(iii) The stochastic forcing $\mathbf{R}$ may be of external origin, its role being solely to regularize the singularities of the invariant density ρ_s associated to the dissipative character of $\mathbf{F}$; account for the thermodynamic fluctuations around the average values of the observables associated with the dissipative perturbation added to the initial conservative dynamics, in which case it should satisfy appropriate fluctuation-dissipation relationships; and account for the interaction between the system and external reservoirs (heat baths, etc). In either case, $\mathbf{R}$ will be modeled as a multi-Gaussian white noise,

$$\begin{gathered}\langle R_i(t)\rangle=0,\\ \langle R_i(t)R_j(t')\rangle=\varepsilon Q_{ij}\delta(t-t'),\end{gathered} \tag{7}$$

Q_{ij} being a positive definite matrix and ε a strength parameter.

Equations (4) and (7) define a Markov process of the diffusion type and induce a Fokker-Planck equation [9] for the evolution of the probability density $\rho(x,t)$

$$\begin{aligned}\frac{\partial\rho}{\partial t}&=-\sum_i\frac{\partial}{\partial x_i}F_i\rho+\frac{\varepsilon}{2}\sum_{ij=1}^{n}Q_{ij}\frac{\partial^2\rho}{\partial x_i\partial x_j}\\ &=\mathcal{L}\rho+\frac{\varepsilon}{2}\sum_{ij}Q_{ij}\frac{\partial^2\rho}{\partial x_i\partial x_j},\end{aligned} \tag{8}$$

where $\mathcal{L}$ is the Liouville operator.

We will often be interested in the properties of Eq. (8) in the ''weak noise'' limit $\varepsilon\ll 1$. In this limit one may seek for solutions of the form [10]

$$\rho(\mathbf{x},t)=Z_\varepsilon^{-1}\exp\left[\frac{1}{\varepsilon}\phi(\mathbf{x},t)+O(1)\right], \tag{9}$$

where Z_ε is the normalization factor, and ϕ is referred to as the stochastic potential. Substituting into Eq. (8) and keeping only dominant terms in ε, in the steady state one obtains

$$\frac{1}{2}\sum_{ij}Q_{ij}\frac{\partial\phi_s}{\partial x_i}\frac{\partial\phi_s}{\partial x_j}=\sum_i F_i\frac{\partial\phi_s}{\partial x_i}. \tag{10}$$

It can be shown for large classes of systems that ϕ_s, and hence the invariant density ρ_s, are smooth as long as ε is not strictly zero [9–11]. This reflects the regularizing action of the stochastic forcing anticipated earlier in the present section. In the noise-free limit ρ becomes singular—essentially a δ-type distribution having the attractor as support.

We notice that the above formulation contains thermostatted systems as a particular case, provided that F_i and Q_{ij} are such that the mean energy is conserved in time. This class of systems will be analyzed in some detail from this standpoint in Sec. IV.

III. INFORMATION ENTROPY AND ITS BALANCE

In a discrete state, stationary stochastic process entropy can be defined uniquely once the Shannon-Khinchin postulates are adopted [12]. It represents the information (amount of data) necessary to localize the state of the system in a phase space cell of linear dimension δ, and is given by

$$S_I=-\sum_i p_i\ln p_i \tag{11}$$

where the index i stands for the state, and p_i is the probability vector. As the resolution δ becomes finer, p_i tends to $\rho\delta$, where ρ is the corresponding density. Equation (11) then shows that S_I contains a singular part in $\ln(1/\delta)$, plus a regular contribution depending solely on ρ. As the singular part is independent of the dynamics, it can be used as reference value and one obtains the continuous version of Eq. (11),

$$S_I = -\int d\mathbf{x}\,\rho(\mathbf{x},t)\ln\rho(\mathbf{x},t). \tag{12}$$

Having a definition of (information) entropy S_I and an evolution equation for ρ, one can now derive a balance equation for S_I, identify entropy productionlike terms bearing the signature of dynamics in phase space, and compare them with the entropy production of irreversible thermodynamics. We first observe, from Eqs. (8) and (12), that

$$\frac{dS_I}{dt} = -\int d\mathbf{x}\left[-\sum_i \frac{\partial}{\partial x_i}(F_i\rho) + \frac{\varepsilon}{2}\sum_{ij} Q_{ij}\frac{\partial^2\rho}{\partial x_i\partial x_j}\right]\ln\rho. \tag{13}$$

The right hand side of this relation can be transformed by performing partial integrations. Dropping boundary terms [13] (a legitimate procedure since the probability density tends rapidly to zero as $|\mathbf{x}|\to\infty$), after some straightforward manipulations one obtains the following form of information entropy balance:

$$\frac{dS_I}{dt} = \int d\mathbf{x}\,\rho\,\mathrm{div}\,\mathbf{F} + \frac{\varepsilon}{2}\sum_{ij} Q_{ij}\int d\mathbf{x}\frac{1}{\rho}\frac{\partial\rho}{\partial x_i}\frac{\partial\rho}{\partial x_j}. \tag{14}$$

The second term in Eq. (14) is positive definite on the grounds of the positive definiteness of the matrix Q_{ij}, while the first one has no definite sign. This suggests identifying the latter with (information) entropy flux and the former with (information) entropy production P_I, given by the relation

$$P_I = \frac{\varepsilon}{2}\sum_{ij} Q_{ij}\int d\mathbf{x}\frac{1}{\rho}\frac{\partial\rho}{\partial x_i}\frac{\partial\rho}{\partial x_j}. \tag{15}$$

A more explicit representation of P_I can be obtained in the steady state, and in the limit $\varepsilon \ll 1$, using expressions (9) and (10). We obtain

$$P_I = \frac{1}{2\varepsilon}\sum_{ij} Q_{ij}\int d\mathbf{x}\,\rho_s\frac{\partial\phi_s}{\partial x_i}\frac{\partial\phi_s}{\partial x_j} = \int d\mathbf{x}\sum_i F_i\frac{\partial\rho_s}{\partial x_i} \tag{16}$$

or, after a partial integration,

$$P_I = -\int d\mathbf{x}\,\rho_s\,\mathrm{div}\,\mathbf{F} = -\overline{\mathrm{div}\,\mathbf{F}}^{\infty} = -\sum_i \sigma_i + O(\varepsilon) > 0, \tag{17}$$

where σ_i are the Lyapunov exponents of the deterministic system [Eqs. (4) in the absence of noise]. We have thus shown, for a very general class of dynamical systems, that information entropy production as defined by Eq. (15) is equal to the negative sum of Lyapunov exponents or equivalently [cf. Eq. (1)] to the rate of phase space volume contraction, plus a correction vanishing with the noise strength [14,15]. This result is rather remarkable, since it would seem at first sight from Eq. (15) that P_I should tend to zero as $\varepsilon\to 0$. The fact that it nevertheless gives a finite contribution in this limit reflects the nonanalytic dependence of the probability density in ε [Eq. (9)].

In short we have established, through P_I, a link between thermodynamically inspired quantities and the quantifiers of the underlying dynamics in phase space, free of the difficulties outlined in Sec. I. Still, no connection with the entropy production of irreversible thermodynamics has been made at this stage, since the distance from equilibrium has not been explicitly displayed. To achieve this we decompose the diffusion term in the Fokker-Planck equation (8) in a new way exhibiting the equilibrium distribution ρ_e, using the identity

$$\frac{\partial^2\rho}{\partial x_i\partial x_j} = \frac{\partial}{\partial x_i}\left[\rho\frac{\partial\ln\rho_e}{\partial x_j}\right] + \frac{\partial}{\partial x_i}\left[\rho_e\frac{\partial}{\partial x_j}\frac{\rho}{\rho_e}\right]. \tag{18}$$

We emphasize that ρ_e is the stationary solution of the full equation (8), in which the parameter μ (included in F_i) is simply set equal to its equilibrium value μ_e. In particular, ρ_e incorporates effects due to the fluctuations. The information entropy balance, Eqs. (13) and (14) now yields

$$\begin{aligned}\frac{dS_I}{dt} = &-\int d\mathbf{x}\ln\rho\left[-\sum_i\frac{\partial}{\partial x_i}(F_i\rho) + \frac{\varepsilon}{2}\sum_{ij}Q_{ij}\frac{\partial}{\partial x_i}\left(\rho\frac{\partial\ln\rho_e}{\partial x_j}\right)\right]\\ &-\int d\mathbf{x}\ln\rho_e\frac{\varepsilon}{2}\sum_{ij}Q_{ij}\frac{\partial}{\partial x_i}\left(\rho_e\frac{\partial}{\partial x_j}\frac{\rho}{\rho_e}\right) + \int d\mathbf{x}\,\rho\frac{\varepsilon}{2}\sum_{ij}Q_{ij}\left(\frac{\partial}{\partial x_i}\ln\frac{\rho}{\rho_e}\right)\left(\frac{\partial}{\partial x_j}\ln\frac{\rho}{\rho_e}\right).\end{aligned} \tag{19}$$

We notice that the first, second, and third integrals in Eq. (19) are of zeroth, first, and second order, respectively, with respect to the deviation from equilibrium. Performing partial integrations as above, one obtains

$$\frac{dS_I}{dt} = \overline{\mathrm{div}\,\mathbf{F}}^{t} + \frac{\varepsilon}{2}\sum_{ij}Q_{ij}\int d\mathbf{x}\,\rho\left[-\frac{\partial\ln\rho_e}{\partial x_i}\frac{\partial\ln\rho_e}{\partial x_j} + 2\frac{\partial\ln\rho}{\partial x_i}\frac{\partial\ln\rho_e}{\partial x_j}\right] + \frac{\varepsilon}{2}\sum_{ij}Q_{ij}\int d\mathbf{x}\,\rho\left(\frac{\partial}{\partial x_i}\ln\frac{\rho}{\rho_e}\right)\left(\frac{\partial}{\partial x_j}\ln\frac{\rho}{\rho_e}\right). \tag{20}$$

This new decomposition of the rate of change of information entropy now features a part P_I'

$$P_I' = \frac{\varepsilon}{2}\sum_{ij} Q_{ij}\int d\mathbf{x}\,\rho\left(\frac{\partial}{\partial x_i}\ln\frac{\rho}{\rho_e}\right)\left(\frac{\partial}{\partial x_j}\ln\frac{\rho}{\rho_e}\right) \geqslant 0, \quad (21)$$

which is both positive definite and of second order in the deviation from equilibrium, thereby fulfilling the principal condition required on entropy production. On the other hand, the first term on the right-hand side of Eq. (20), $\overline{\mathrm{div}\,F^t}$, has no definite sign and contains, in principle, contributions of all orders in the deviation from equilibrium. In the steady state, $dS_I/dt=0$, and the contribution of this term and of the second one in Eq. (20) must cancel that of P_I'. The role of this latter term in this balance is, then, to remove the contributions of all but second orders in the deviation from equilibrium contained in $\overline{\mathrm{div}\,\mathbf{F}^t}$. We may therefore write, in the steady state

$$P_I' = -\overline{\mathrm{div}\,\mathbf{F}^\infty} - (\text{terms of 0th and 1st order in } h) \quad (22)$$

or [cf. Eq. (17)]

$$P_I' = -\sum_i \sigma_i - (\text{terms of 0th and 1st order in } h). \quad (23)$$

This establishes a connection between irreversible thermodynamics on the one side, and phase space dynamics on the other. At this stage this connection cannot be made more explicit, as our analysis encompasses a very wide class of dynamical systems. In the next two sections more explicit forms of entropy balance are derived for the specific cases of thermostatted systems and mesoscopic systems.

IV. THERMOSTATTED SYSTEMS

As mentioned in Sec. I, thermostatted systems have recently attracted considerable attention since they provide an interesting way to incorporate the nonequilibrium constraints in the form of an external ''mechanical'' force added to the equations of evolution of the microscopic degrees of freedom [1,16–18].

The approach to thermostatted systems developed in this section is based on the idea that thermostatting should already be present in equilibrium. This entails that the evolution operator $\mathbf{F}(\mathbf{x},\mu)$ should remain dissipative even for $\mu=\mu_e$. To express the action of the nonequilibrium constraint, we decompose the deterministic part $\mathbf{F}$ in Eq. (4) into the sum of a contribution $\mathbf{F}_0=\mathbf{F}(\mathbf{x},\mu_e)$ to which $\mathbf{F}$ reduces in the absence of nonequilibrium constraint [$h=0$ in Eq. (6)] and of a contribution $h(\partial\mathbf{F}/\partial\mu)_{\mu_e}=h\mathbf{F}_1$ associated with the action of the constraint. Equation (4) then becomes

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}_0(\mathbf{x}) + h\mathbf{F}_1(\mathbf{x}) + \mathbf{R}(t). \quad (24)$$

The variables x_i now represent the coordinates $\mathbf{q}_i$ and momenta $\mathbf{p}_i$ of a system of particles in contact with a reservoir. The equilibrium part $\mathbf{F}_0$ together with the fluctuating forces $\mathbf{R}$ ensure that in the limit $h=0$ the system is driven irreversibly to canonical equilibrium.

The Fokker-Planck equation associated with Eq. (24) reads

$$\frac{\partial\rho}{\partial t} = -\sum_i \frac{\partial}{\partial x_i}\left[\left(F_{0i} - \frac{1}{2}\sum_j Q_{ij}\frac{\partial\ln\rho_e}{\partial x_j}\right)\rho\right] - h\sum_i \frac{\partial}{\partial x_i}(F_{1i}\rho) + \frac{1}{2}\sum_{ij} Q_{ij}\frac{\partial}{\partial x_i}\left(\rho_e\frac{\partial}{\partial x_j}\frac{\rho}{\rho_e}\right) \quad (25)$$

where the contribution of the diffusion part has been decomposed as in Eq. (18). In equilibrium, $h=0$ and $\rho=\rho_e$. The second and third terms on the right-hand side of Eq. (25) then vanish identically, entailing that the first term must also vanish. This imposes a relation between the parameters appearing in the functions F_{0i} and the matrix Q_{ij}, which can be looked at as the manifestation of a fluctuation-dissipation type of theorem (we assume for simplicity that Q_{ij} is not affected by the nonequilibrium constraint). More explicitly, one has

$$-\sum_i \frac{\partial}{\partial x_i}(\phi_i\rho_e) = 0 \quad (26)$$

where the ''effective'' vector field ϕ_i governing the dynamics around equilibrium is given by

$$\phi_i = F_{0i} - \frac{1}{2}\sum_j Q_{ij}\frac{\partial\ln\rho_e}{\partial x_j}. \quad (27)$$

Now Eq. (26) must be compatible with the equilibrium limit of the full-scale (microscopic) Liouville equation in the absence of constraint,

$$\rho_e \sim \exp(-\beta H), \quad (28)$$

H being the total energy. We therefore stipulate that ϕ_i must have a symplectic structure and, in particular, be divergence free:

$$\mathrm{div}\,\phi = 0. \quad (29)$$

The underlying dynamics associated with the drift term in Eq. (25) is, therefore, time reversible and phase space volume conserving, and the modified diffusion term in this equation provides the proper way to account for the fluctuations around such an equilibrium conservative dynamics. Finally, the term in h in Eq. (25) expresses the nonequilibrium part of the dynamics, which will be modeled as a dissipative (phase space volume-contracting) process,

$$\overline{\operatorname{div}\mathbf{F}_1}^{\,t}<0 \qquad t\geqslant t_0. \tag{30}$$

We come now to the information entropy balance. Differentiating Eq. (12) with respect to time and using Eq. (25) we obtain

$$\frac{dS_I}{dt}=-\frac{d}{dt}\int d\mathbf{x}\,\rho\ln\rho_e-\int d\mathbf{x}\ln\frac{\rho}{\rho_e}\Bigg[-\sum_i\frac{\partial}{\partial x_i}(\phi_i\rho)-h\sum_i\frac{\partial}{\partial x_i}(F_{1i}\rho)+\frac{1}{2}\sum_{ij}Q_{ij}\frac{\partial}{\partial x_i}\left(\rho_e\frac{\partial}{\partial x_j}\frac{\rho}{\rho_e}\right)\Bigg]. \tag{31}$$

The new element is now that in isoenergetically thermostatted systems the term in d/dt vanishes identically, owing to the conservation of the mean value of total energy H [cf. Eq. (28)]. The remaining part of Eq. (31) is then automatically of second order in the deviation from equilibrium, in particular since the action of $-\Sigma_i(\partial/\partial x_i)\phi_i$ on ρ_e gives zero: the zeroth and first order terms in Eq. (23) are therefore absent. We may give to this part a more explicit form by performing partial integration. Noticing that the action of the part in ϕ_i gives a vanishing result, one obtains

$$\frac{dS_I}{dt}=h^2\int d\mathbf{x}\,\delta\rho\,\operatorname{div}\mathbf{F}_1+h^2\int d\mathbf{x}\left(\sum_i F_{1i}\frac{\partial\ln\rho_e}{\partial x_i}\right)\delta\rho+\frac{\varepsilon}{2}\sum_{ij}Q_{ij}\int d\mathbf{x}\rho\left(\frac{\partial}{\partial x_i}\ln\frac{\rho}{\rho_e}\right)\left(\frac{\partial}{\partial x_j}\ln\frac{\rho}{\rho_e}\right), \tag{32}$$

where $h\,\delta\rho=\rho-\rho_e$. We thus recover the entropy production term P_I' [Eq. (21)], together with a more explicit expression of the remaining, entropy flux like terms, J_I', as compared to Eq. (20):

$$J_I'=h^2\int d\mathbf{x}\,\delta\rho\,\operatorname{div}\mathbf{F}_1-\beta h^2\int d\mathbf{x}\sum_i F_{1i}\frac{\partial H}{\partial x_i}\delta\rho. \tag{33}$$

Here the first part represents the rate of phase-space volume contraction to the second order, whereas the second part can be viewed as the average of the work per unit time of the external forcings acting (tangentially) along the different degrees of freedom i. In the steady state,

$$P_I'=-J_I', \tag{34}$$

providing an explicit relation between irreversible thermodynamics and phase space dynamics.

As an illustration of the foregoing we consider Brownian motion in an external field [19],

$$\frac{dv}{dt}=-\zeta v+\frac{eE}{m}+R(t), \tag{35}$$

where m is the mass, e is the charge, and the coefficient ζ expresses the effect of friction exerted on the particle by the host fluid, which acts like a heat bath at constant temperature T. This can thus be viewed as a thermostatted system which remains dissipative when the nonequilibrium constraint vanishes. The correspondence with the general form (24) leads to the identification $F_0=-\zeta v$, $F_1=eE/m$.

The Fokker-Planck equation corresponding to Eq. (35) can be solved straightforwardly, yielding

$$\rho_e=\left(\frac{m}{2\pi kT}\right)^{1/2}e^{-(mv^2/2kT)}, \tag{36}$$

where use was made of the fluctuation-dissipation relation [9,19], $(\varepsilon/2)Q=\zeta kT/m$.

The flux term J_I' in Eq. (33) becomes

$$J_I'=-\frac{1}{kT}\int_{-\infty}^{\infty}dv\,eEv(\rho-\rho_e), \tag{37}$$

where the integrand represents the work per unit time performed on the particle by the external force. Hence one obtains, in the steady state,

$$J_I'=-\frac{e^2E^2}{\zeta kT}, \quad P_I'=-J_I'=\frac{e^2E^2}{\zeta kT} \tag{38}$$

which is exactly the entropy production of irreversible thermodynamics for this system.

It is worth noting that the "effective" vector field ϕ corresponding to this dynamical system vanishes identically due to the absence of inertial terms in the field-free limit of Eq. (35). Indeed, using the above given explicit forms of ρ_e and Q, one finds, from Eq. (27),

$$\phi=-\frac{\zeta}{m}v-Q\frac{\partial}{\partial v}\left(-\frac{mv^2}{2kT}\right)=0. \tag{39}$$

The Fokker-Planck equation for this system reduces thus actually to the last two terms of Eq. (25),

$$\frac{\partial\rho}{\partial t}=-\frac{eE}{m}\frac{\partial\rho}{\partial v}+\frac{\zeta kT}{m^2}\frac{\partial}{\partial v}\left(\rho_e\frac{\partial}{\partial v}\frac{\rho}{\rho_e}\right). \tag{40}$$

A similar structure will arise in all problems involving purely dissipative evolution laws.

V. MESOSCOPIC SYSTEMS

We next turn to the case where $\mathbf{x}$ stands for a set of macroscopic observables, and $\mathbf{R}$ for the thermodynamic fluctuations. In the small noise limit $\varepsilon\ll1$ considered in Sec. III the density ρ is expected to be peaked sharply around the attractor of the deterministic (noiseless) evolution equations. We express this by decomposing $\mathbf{x}$ as

$$\mathbf{x}=\overline{\mathbf{x}}+\delta\mathbf{x}, \qquad \frac{|\delta\mathbf{x}|}{|\overline{\mathbf{x}}|}\ll1 \tag{41}$$

and by limiting the expansion of the rate function $\mathbf{F}(\mathbf{x},\mu)$ in Eq. (4) around $\overline{\mathbf{x}}$ to its linear terms,

$$\dot{\delta\mathbf{x}}=\mathbf{l}\delta\mathbf{x}+\mathbf{R}(t), \tag{42}$$

where

$$l_{ij}=\left(\frac{\partial F_i}{\partial x_j}\right)_{\overline{x}}. \tag{43}$$

Here $\overline{x}$ is the macroscopic state (average or more generally most probable value of the probability density) evolving according to

$$\dot{\mathbf{x}}=\mathbf{F}(\overline{\mathrm{x}},\mu). \tag{44}$$

The Fokker-Planck equation induced by Eq. (42) then reads

$$\frac{\partial\rho}{\partial t}=-\sum_{ij}\frac{\partial}{\partial\delta x_i}l_{ij}\delta x_j\rho+\frac{\varepsilon}{2}\sum_{ij}Q_{ij}\frac{\partial^2\rho}{\partial\delta x_i\partial\delta x_j}. \tag{45}$$

Inasmuch as the macroscopic steady state $\overline{\mathbf{x}_s}$ is stable, Eq. (45) admits a stationary solution in the form of a multivariate Gaussian distribution

$$\rho(\delta\mathbf{x},t)=\frac{\sqrt{g/\varepsilon}}{(2\pi)^{n/2}}\exp\left[-\frac{1}{2\varepsilon}\sum_{ij}g_{ij}\delta x_i\delta x_j\right] \tag{46}$$

where the matrix $\mathbf{g}$ is given by [20]

$$\mathbf{l}\mathbf{g}^{-1}+(\mathbf{l}\mathbf{g}^{-1})^T=-\mathbf{Q}, \tag{47}$$

g being its determinant.

So far we have not specified the thermodynamic status of our system and, in particular, its distance from thermodynamic equilibrium. Operationally this distance is monitored by the control parameter μ present in the evolution laws [Eq. (4)], which may account for the interaction of the system with external reservoirs and/or for the direct action of an external field. At equilibrium ($\mu=\mu_e$), Eq. (46) reduces to

$$\rho_e(\delta\mathbf{x}_e)=\frac{\sqrt{g^e/\varepsilon}}{(2\pi)^{n/2}}\exp\left[-\frac{1}{2\varepsilon}\sum_{ij}g_{ij}^e\delta x_i^e\delta x_j^e\right] \tag{48}$$

where g_{ij}^e is related to the deviation ΔS of thermodynamic entropy from its equilibrium value due to a fluctuation through [19]

$$g_{ij}^e=-\left(\frac{\partial^2\Delta S}{\partial\delta x_i\partial\delta x_j}\right). \tag{49}$$

Here we are interested in the linear response to a weak nonequilibrium constraint h,

$$\rho=\rho_e+h\,\delta\rho+o(h^2),$$

$$\mu=\mu_e+h,\quad\left|\frac{h}{\mu_e}\right|\ll 1. \tag{50}$$

As a rule, the effect of the constraint will be twofold.

(i) The macroscopic state $\overline{\mathbf{x}}$ is shifted from the equilibrium value $\mathbf{x}_e$,

$$\overline{\mathbf{x}}=\mathbf{x}_e+h\mathbf{x}^{(1)}+\cdots; \tag{51}$$

hence

$$\delta\mathbf{x}=\delta\mathbf{x}_e-h\mathbf{x}^{(1)}. \tag{52}$$

Substituting Eq. (51) into Eq. (44), and expanding around $\mathbf{x}_e$ and μ_e to first order in h yields

$$\mathbf{x}^{(1)}=-\ell_e^{-1}\left(\frac{\partial\mathbf{F}}{\partial\mu}\right)_e. \tag{53}$$

(ii) The matrix $\mathbf{g}$ and its determinant g will deviate from their equilibrium values

$$\mathbf{g}=\mathbf{g}_e+h\mathbf{g}^{(1)},$$

$$g=g_e+hg^{(1)}, \tag{54}$$

as a result of the nonequilibrium corrections to the Jacobian matrix $\mathbf{l}$ and to the noise correlation matrix Q in Eq. (47):

$$\mathbf{l}=\mathbf{l}_e+h\mathbf{l}^{(1)}+\cdots,$$

$$\mathbf{Q}=\mathbf{Q}_e+h\mathbf{Q}^{(1)}+\cdots. \tag{55}$$

Carrying out these expansions systematically in Eqs. (46) and (47), we finally obtain

$$\delta\rho=\left(\frac{g^{(1)}}{2g_e}+\frac{1}{2\varepsilon}\sum_{ij}g_{ij}^e(\delta x_i^e x_j^{(1)}+\delta x_j^e x_i^{(1)})-\frac{1}{2\varepsilon}\sum_{ij}g_{ij}^{(1)}\delta x_i^e\delta x_j^e\right)\rho_e. \tag{56}$$

We are now in the position to evaluate the information entropy production P_I' [Eq. (21)]. Adopting the Onsager definition of the thermodynamic force X_i associated with x_i,

$$X_i=\frac{\partial\Delta S}{\partial x_i}=-\sum_k g_{ik}^e x_k, \tag{57}$$

and noting that the part Q_{ij}^e of Q_{ij} is twice the Onsager matrix L_{ij} of phenomenological coefficients [9] we obtain, to the leading order in the noise strength ε,

$$P_I'=\frac{1}{\varepsilon}\sum_{ij}L_{ij}\overline{X}_i^{(1)}\overline{X}_j^{(1)}+O(h^3,\varepsilon^0). \tag{58}$$

This is nothing but the Gibbsian form of entropy production of irreversible thermodynamics [19]. The factor $1/\varepsilon$ accounts for the extensivity of the entropy production since it is proportional to the volume of the system. Notice that the connection with phase space dynamics is now less explicit than in Sec. IV; see Eqs. (21) and (22).

VI. CONCLUSIONS

We have developed a thermodynamic approach to the class of dynamical systems amenable to a Fokker-Planck type of description based on the balance equation of information entropy. Entropy flux and entropy productionlike terms depending on the characteristics of the dynamics in phase space have been identified, and an explicit relation [Eq. (15)] linking information entropy production to the rate of phase space volume contraction has been derived. Connections with irreversible thermodynamics have subsequently been explored on two case studies pertaining to thermostatted and to mesoscopic systems by displaying explicitly the distance from equilibrium. For the class of thermostatted systems we showed, without invoking an extrinsic conservation law between the system and the reservoir, that information entropy production is given by the negative sum of the rate of phase space volume contraction to the second order, and the average of the work per unit time of the external forcings. An explicit example pertaining to Brownian motion was worked out to illustrate this relation.

Our principal motivation for augmenting the deterministic description by the addition of stochastic forcings is that nonequilibrium constraints reflect the interaction of a system with external reservoirs. Such an interaction involves, as a rule, a reduced description of the reservoirs; it is therefore most naturally modeled by a dissipative term, in which case it also needs to be complemented by explicit consideration of the fluctuations. This procedure which in many respects resembles classical coarse graining [21,22] leads, for free, to a regularization of the invariant probability densities. It is worth noting that this latter is not necessarily achieved by the noise inherent in a computer simulation of the underlying system. Furthermore, this procedure introduces a source term in the entropy balance, counteracting in the steady state the sink term which was the only one appearing in Eq. (3). In the absence of the nonequilibrium constraint this description generates quite naturally the correct canonical equilibrium limit. In our view thermostatting should already be active in equilibrium, and this can only be achieved if the evolution operator $\mathbf{F}(\mathbf{x},\mu_e)$ is dissipative. It is only at the level of the ''effective'' vector field ϕ [Eq. (27)] that the conservative character of the underlying microscopic dynamics will show up.

Future work in this area should aim at establishing the link between irreversible thermodynamics and phase space dynamics for more representative systems and on a still more explicit basis. For instance, in most realistic systems, Lyapunov exponents and contraction rates fluctuate considerably along the invariant manifolds. The repercussions of these fluctuations on thermodynamic properties would certainly be worth elucidating. Of special interest are also are multivariate, spatially extended systems possessing a large number of Lyapunov exponents. The extent to which all the exponents contribute to macroscopic level properties like entropy production is largely unknown, and one might advance that only a few of them—presumably the slowest ones—would play an important role.

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