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Temporal Behavior of the Conditional and Gibbs' Entropies

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We study the temporal approach to equilibrium of the Gibbs' and conditional entropies for stochastic systems in the presence of white noise. The conditional entropy will either remain constant or monotonically increase to its maximum of zero. However, the Gibbs' entropy may have a variety of patterns of approach to its final value ranging from a monotone increase or decrease to an oscillatory approach. We have illustrated all of these behaviors using examples in which both entropy dynamics can be determined analytically.

KEY WORDS: conditional entropy, Gibbs' entropy, asymptotic stability, Ornstein-Uhlenbeck process, noisy harmonic oscillator

1. INTRODUCTION

A variety of measures of dynamic behavior carry the name of entropy. Two have proved to be especially intriguing in the examination of the temporal evolution of dynamical systems when considered from an ensemble point of view. One of these is known as the conditional entropy. Convergence properties of the conditional entropy have been extensively studied because 'entropy methods' have been known for some time to be useful for problems involving questions related to convergence of solutions in partial differential equations.[1–6] Their utility can be traced, in some instances, to the fact that the conditional entropy may serve as a Liapunov functional.[7] Another type of entropy is the Gibbs' entropy, which is

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strongly related to an extension of the equilibrium entropy that was introduced by Gibbs.[8] This has been considered by a number of authors recently, specifically in Ruelle,[9,10] Nicolis and Daems,[11] Daems and Nicolis[12] and Bag *et al.*,[13,14] Bag.[15–17]

Here we compare and contrast the temporal evolution of the conditional and Gibbs' entropies in a variety of dynamical settings. Our primary considerations are stochastic systems with additive white noise. The organization of the paper is as follows. Section 2 gives some basic background, definition of steady state Gibbs' entropy, and extension of this to time dependent situations. In Sec. 3 we examine the temporal behavior of the conditional entropy in asymptotically stable systems, and contrast these with the behavior of the Gibbs' entropy. These considerations are illustrated in Sec. 4 with two detailed examples drawn from dynamical systems perturbed by noise. The paper concludes with a summary in Sec. 5.

2. GIBBS' AND CONDITIONAL ENTROPIES

Let X be a phase space and μ a reference measure on X. Denote the corresponding set of densities by $\mathcal{D}(X)$, or $\mathcal{D}$ when there will be no ambiguity, so $f \in \mathcal{D}$ means $f \geq 0$ and $\int_X f(x)\,dx = 1$ (for integrals with respect to the reference measure we use the notation $\int f(x)\,dx$ rather than $\int f(x)\,d\mu(x)$).

In his seminal work Gibbs,[8] assuming the existence of a system steady state density f_* on the phase space X, introduced the concept of the index of probability given by $\log f_*(x)$ where "log" denotes the natural logarithm. He then identified the entropy in a steady state situation with the average of the index of probability

$$H_G(f_*) = -\int_X f_*(x) \log f_*(x)\,dx, \tag{2.1}$$

and we call this the *equilibrium or steady state Gibbs' entropy*. If the equilibrium entropy is to be an extensive quantity (in accord with experimental evidence) then Definition 2.1 is unique up to a multiplicative constant.[18,19]

We extend the definition of the steady state Gibbs' entropy to time dependent (non-equilibrium) situations and say that the *time dependent Gibbs' entropy* of a density $f(t,x)$ is defined by

$$H_G(f) = -\int_X f(t,x) \log f(t,x)\,dx. \tag{2.2}$$

We define the conditional entropy as[20]

$$H_c(f|f_*) = -\int_X f(t,x) \log \frac{f(t,x)}{f_*(x)}\,dx. \tag{2.3}$$

It is variously known as the Kullback-Leibler or relative entropy,[1] the relative Boltzmann entropy,[21,22] or the specific relative entropy,[23] and has been related to the free energy.[5,6,24] If there is a convergence $\lim_{t\to\infty} f(t,x) = f_*(x)$ in some sense (which we will make totally precise in Sec. 3) then $\lim_{t\to\infty} H_c(f|f_*) = 0$.

3. ASYMPTOTIC STABILITY AND CONDITIONAL ENTROPY

Let $\{P^t\}$ be a family of Markov operators on $L^1(X)$, i.e. $P^t f_0 \geq 0$ for an initial density $f_0 \geq 0$, $\int P^t f_0(x)\,dx = \int f_0(x)\,dx$, and $P^{t+s} f_0 = P^t(P^s f_0)$. If the latter property holds for $t, s \in \mathbf{R}$, then $\{P^t\}_{t\in\mathbf{R}}$ is a group of Markov operators. If it holds only for $t, s \in \mathbf{R}^+$, then $\{P^t\}_{t\geq 0}$ is a semigroup of Markov operators. If there is a density f_* such that $P^t f_* = f_*$ for all $t > 0$, f_* is called a stationary density of P^t.

Our first result shows that the conditional entropy is nondecreasing.

Theorem 1. ([26]). *Let P^t be a family of Markov operators on $L^1(X)$ and f_* be the stationary density. Then for every density f_0 the conditional entropy $H_c(P^t f_0|f_*)$ is a nondecreasing function of t.*

Our next result from Ref. 25 shows that when P^t satisfies the group property the conditional entropy is uniquely determined by the system preparation and does not change with time. This is formalized in

Theorem 2. ([25], Theorem 3.2). *If P^t is a group of Markov operators and has a stationary density f_*, then the conditional entropy is constant and equal to the value determined by f_* and the choice of the initial density f_0 for all time t. That is,*

$$H_c(P^t f_0|f_*) \equiv H_c(f_0|f_*)$$

for all t.

For a given density f_0 the conditional entropy $H_c(P^t f_0|f_*)$ is bounded above by zero. Thus we know that it has a limit as $t \to \infty$. Our next result connects the temporal convergence properties of H_c with those of P^t. A semigroup of Markov operators P^t on $L^1(X)$ is said to be *asymptotically stable*[20] if there is a stationary density f_* of P^t such that for all initial densities f_0

$$\lim_{t\to\infty} P^t f_0 = f_*$$

(here the limit denotes convergence in $L^1(X)$).

The next result holds for situations when P^t satisfies the semigroup property.

Theorem 3. ([27], Theorem 1). *Let P^t be a semigroup of Markov operators on $L^1(X)$ and f_* be the stationary density. Then*

$$\lim_{t\to\infty} H_c(P^t f_0 | f_*) = 0$$

for all f_0 with $H_c(f_0|f_*) > -\infty$ if and only if P^t is asymptotically stable.

Theorem 3 shows that asymptotic stability is necessary and sufficient for the convergence of H_c to zero. A consequence of the convergence of the conditional entropy to zero is that

$$\lim_{t\to\infty} \int h(x) P^t f_0(x)\, dx = \int h(x) f_*(x)\, dx$$

for any measurable function h for which the integral

$$\int e^{rh(x)} f_*(x)\, dx$$

is finite for all r in some neighborhood of zero [28, Lemma 3.1]. Since the conditional and Gibbs' entropies are related by

$$H_G(P^t f_0) = H_c(P^t f_0 | f_*) - \int P^t f_0(x) \log f_*(x)\, dx, \tag{3.1}$$

Theorem 3 implies

Theorem 4. *Let P^t be an asymptotically stable semigroup of Markov operators on $L^1(X)$ with a stationary density f_* such that $\int f_*^{1+r}(x)\, dx < \infty$ for all r in some neighborhood of zero. Then*

$$\lim_{t\to\infty} H_G(P^t f_0) = H_G(f_*)$$

for all f_0 with $H_c(f_0|f_*) > -\infty$.

These theorems are very general in their statements about the behavior of the conditional and Gibbs' entropies. Namely, Theorem 2 tells us that when the dynamics is such that P^t is a group (we have a dynamical system) the conditional entropy will be constant and fixed by the initial value of f_0. However, when P^t is an asymptotically stable semigroup then Theorems 3 and 4 respectively guarantee the convergence of the conditional entropy to its maximal value of zero and the Gibbs' entropy to its equilibrium value.

4. ENTROPY BEHAVIOR AND THE EFFECTS OF NOISE IN CONTINUOUS TIME SYSTEMS

In this section, we consider the behavior of the entropies $H_G(P^t f_0)$ and $H_c(P^t f_0|f_*)$ when the dynamics are described by the stochastically perturbed system

$$\frac{dx_i}{dt} = F_i(x) + \sum_{j=1}^{d} \sigma_{ij}(x)\xi_j, \qquad i = 1, \ldots, d \tag{4.1}$$

with the initial conditions $x_i(0) = x_{i,0}$. $\sigma_{ij}(x)$ is the amplitude of the stochastic perturbation and $\xi_j = \frac{dw_j}{dt}$ is a white noise term that is the derivative of a Wiener process. We interpret Eq. (4.1) using Itô calculus rather than Stratonovich calculus. (For the differences see Refs. 20, 29, 30. If the σ_{ij} are independent of x then the Itô and the Stratonovich approaches yield identical results.)

The *Fokker-Planck equation* governing the evolution of the density function $f(t, x)$ is given by

$$\frac{\partial f}{\partial t} = -\sum_{i=1}^{d} \frac{\partial[F_i(x)f]}{\partial x_i} + \frac{1}{2}\sum_{i,j=1}^{d} \frac{\partial^2[a_{ij}(x)f]}{\partial x_i \partial x_j} \tag{4.2}$$

where

$$a_{ij}(x) = \sum_{k=1}^{d} \sigma_{ik}(x)\sigma_{jk}(x).$$

If $k(t, x, x_0)$ is the fundamental solution of the Fokker-Planck equation, i.e. for every x_0 the function $(t, x) \mapsto k(t, x, x_0)$ is a solution of the Fokker-Planck equation with the initial condition $\delta(x - x_0)$, then the general solution $f(t, x)$ of the Fokker-Planck Eq. (4.2) with the initial condition $f(x, 0) = f_0(x)$ is given by

$$f(t, x) = \int k(t, x, x_0) f_0(x_0)\, dx_0, \tag{4.3}$$

and defines a Markov semigroup by $P^t f_0(x) = f(t, x)$. If a stationary (steady state) density $f_*(x)$ exists, it is the stationary solution of Eq. (4.2):

$$-\sum_{i=1}^{d} \frac{\partial[F_i(x)f]}{\partial x_i} + \frac{1}{2}\sum_{i,j=1}^{d} \frac{\partial^2[a_{ij}(x)f]}{\partial x_i \partial x_j} = 0. \tag{4.4}$$

There are a number of results giving conditions such that the general solution $f(t, x)$ of the Fokker Planck equation is asymptotically stable and thus the conditional entropy evolves monotonically to zero, e.g. Theorem 11.9.1 in Ref. 20. In particular, assume that the stationary density is of the form

$$f_*(x) = e^{-B(x)}.$$

From Theorem 3 it follows that

$$\lim_{t\to\infty} H_c(f|f_*) = 0$$

and from Theorem 4 that

$$\lim_{t\to\infty} H_G(f) = H_G(f_*)$$

for all f_0 with $H_c(f_0|f_*) > -\infty$ provided that $\int e^{-(1+r)B(x)}dx < \infty$ for r in some neighborhood of zero.

We now turn to a comparision of the rate of change of H_G and H_c with expressions that have recently been derived by Daems and Nicolis[12] and Bag.[15] Differentiating Eq. (2.2) for the Gibbs' entropy yields

$$\frac{dH_G}{dt} = \int f\left(\sum_i \frac{\partial F_i(x)}{\partial x_i} - \frac{1}{2}\sum_{i,j}\frac{\partial^2 a_{ij}(x)}{\partial x_i \partial x_j}\right) dx \\ +\frac{1}{2}\int \frac{1}{f}\sum_{i,j=1}^{d} a_{ij}(x)\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}\, dx. \tag{4.5}$$

If the a_{ij} are independent of x then we obtain

$$\frac{dH_G}{dt} = \int f\sum_i \frac{\partial F_i(x)}{\partial x_i}\, dx + \frac{1}{2}\sum_{i,j=1}^{d} a_{ij}\int \frac{1}{f}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}\, dx. \tag{4.6}$$

As pointed out in Daems and Nicolis [12, Eq. 14], the first term is of indeterminant sign, while the second is positive definite so the temporal behavior of the Gibbs' entropy in this system is unclear. It has become customary, c.f. Daems and Nicolis,[12] Bag *et al.*,[13,14] Bag,[15–17] Majee and Bag[31] to refer to the first term in Eq. (4.5) as the 'entropy flux' and the second term as the 'entropy production.'

Differentiating Eq. (2.3) with respect to time, and using Eq. (4.2) with integration by parts along with the fact that since f_* is a stationary density it satisfies (4.4), we obtain

$$\frac{dH_c}{dt} = \frac{1}{2}\int \left(\frac{f_*^2}{f}\right)\sum_{i,j=1}^{d} a_{ij}(x)\frac{\partial}{\partial x_i}\left(\frac{f}{f_*}\right)\frac{\partial}{\partial x_j}\left(\frac{f}{f_*}\right) dx. \tag{4.7}$$

Since the matrix $(a_{ij}(x))$ is nonnegative definite, one concludes that $\frac{dH_c}{dt} \geq 0$. Using the identity

$$\frac{\partial}{\partial x_i}\left(\log \frac{f}{f_*}\right) = \frac{f_*}{f}\frac{\partial}{\partial x_i}\left(\frac{f}{f_*}\right),$$

we can rewrite Eq. (4.7) in the equivalent form

$$\frac{dH_c}{dt} = \frac{1}{2}\int f \sum_{i,j=1}^{d} a_{ij}(x)\frac{\partial}{\partial x_i}\left(\log \frac{f}{f_*}\right)\frac{\partial}{\partial x_j}\left(\log \frac{f}{f_*}\right) dx. \tag{4.8}$$

Daems and Nicolis [12, Eq. 21] and Bag [15, Eq. 43] have derived the right hand side of Eq. (4.8) by rewriting the second term on the right hand side of Eq. (4.6) and integrating by parts. Both refer to the result as entropy production.

4.1. The One Dimensional Case

In a one dimensional system ($d = 1$) the stochastic differential Eq. (4.1) becomes

$$\frac{dx}{dt} = F(x) + \sigma(x)\xi, \tag{4.9}$$

where ξ is a (Gaussian distributed) perturbation with zero mean and unit variance, and $\sigma(x)$ is the amplitude of the perturbation. The corresponding Fokker-Planck Eq. (4.2) is

$$\frac{\partial f}{\partial t} = -\frac{\partial[F(x)f]}{\partial x} + \frac{1}{2}\frac{\partial^2[\sigma^2(x)f]}{\partial x^2}. \tag{4.10}$$

If stationary solutions $f_*(x)$ of (4.10) exist, they are defined by $P^t f_* = f_*$ for all t and given as the generally unique (up to a multiplicative constant) solution of

$$-\frac{\partial[F(x)f_*]}{\partial x} + \frac{1}{2}\frac{\partial^2[\sigma^2(x)f_*]}{\partial x^2} = 0. \tag{4.11}$$

The integrable solution is given by

$$f_*(x) = \frac{K}{\sigma^2(x)} \exp\left[\int^x \frac{2F(z)}{\sigma^2(z)}\, dz\right], \tag{4.12}$$

where $K > 0$ is a normalizing constant and the semigroup P^t is asymptotically stable.

It is known [27, Sec. 4] that under relatively mild conditions there exists a constant $\lambda > 0$ such that

$$H_c(P^t f_0 | f_*) \geq e^{-2\lambda t} H_c(f_0 | f_*).$$

Specific examples of $\sigma(x)$ and $F(x)$ for which one can determine the solution $f(t,x)$ of Eq. (4.10) are few. One is an Ornstein-Uhlenbeck process which we consider in our next example.

Example 1. In considering the Ornstein-Uhlenbeck process, developed in thinking about perturbations to the velocity of a Brownian particle, we denote the dependent variable by v so $\sigma(v) \equiv \sigma$ a constant, and $F(v) = -\gamma v$ with $\gamma \geq 0$. Now Eq. (4.9) becomes

$$\frac{dv}{dt} = -\gamma v + \sigma\xi$$

with the Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \frac{\partial[\gamma v f]}{\partial v} + \frac{\sigma^2}{2}\frac{\partial^2 f}{\partial v^2}.$$

The unique stationary solution is

$$f_*(v) = \frac{e^{-\gamma v^2/\sigma^2}}{\int_{-\infty}^{+\infty} e^{-\gamma v^2/\sigma^2} dv} = \sqrt{\frac{\gamma}{\pi\sigma^2}}\, e^{-\gamma v^2/\sigma^2}.$$

If the initial density f_0 is a Gaussian of the form

$$f_0(v) = \frac{1}{\bar{\sigma}\sqrt{2\pi}} \exp\left\{-\frac{(v-\bar{v})^2}{2\bar{\sigma}^2}\right\}$$

where $\bar{\sigma} > 0$ and $\bar{v} \in \mathbf{R}$, then

$$P^t f_0(v) = \frac{1}{\sigma_t\sqrt{2\pi}} \exp\left\{-\frac{(v-\bar{v}(t))^2}{2\sigma_t^2}\right\}$$

wherein

$$\sigma_t^2 = \sigma_*^2 + (\bar{\sigma}^2 - \sigma_*^2)\, e^{-2\gamma t}$$

with $\sigma_*^2 = \sigma^2/2\gamma$ and

$$\bar{v}(t) = \bar{v}\, e^{-\gamma t}.$$

The Gibbs' entropy is

$$H_G(P^t f_0) = \log \sigma_t \sqrt{2\pi} + \frac{1}{2}.$$

Also

$$\int_{-\infty}^{+\infty} P^t f_0(x) \log f_*(x) dx = -\log \sigma_* \sqrt{2\pi} - \frac{1}{2}\frac{\sigma_t^2}{\sigma_*^2},$$

so

$$H_c(P^t f_0|f_*) = \frac{1}{2}\log\left[\frac{\sigma_t^2}{\sigma_*^2}\right] + \frac{1}{2}\left[1 - \frac{\sigma_t^2}{\sigma_*^2}\right]$$
$$= \frac{1}{2}\log\left\{1 + e^{-2\gamma t}\left[\frac{\bar{\sigma}^2}{\sigma_*^2} - 1\right]\right\}$$
$$-\frac{1}{2}e^{-2\gamma t}\left[\frac{\bar{\sigma}^2}{\sigma_*^2} - 1\right].$$

We may examine how the two different types of entropy behave. Although the conditional entropy $H_c(P^t f_0|f_*)$ is an increasing function of time, this is not the case with the Gibbs' entropy, for

$$\frac{dH_G(P^t f_0)}{dt}\begin{cases} > 0 & \text{for } \bar{\sigma}^2 < \sigma_*^2 \\ = 0 & \text{for } \bar{\sigma}^2 = \sigma_*^2 \\ < 0 & \text{for } \bar{\sigma}^2 > \sigma_*^2, \end{cases}$$

implying that the evolution of the Gibbs' entropy in time is a function of the statistical properties ($\bar{\sigma}^2$) of the initial ensemble. All of these conclusions concerning the dynamics of $H_G(P^t f_0)$ are implicit in the work of Bag[(15)] but not explicitly stated.

Similar effects can be observed for the Rayleigh process considered in [27, Sec. 4].

4.2. Multidimensional Ornstein-Uhlenbeck Process

Consider the multidimensional Ornstein-Uhlenbeck process

$$\frac{dx}{dt} = Fx + \Sigma\xi, \tag{4.13}$$

where F is a $d \times d$ matrix, Σ is a $d \times d$ matrix and ξ is d dimensional vector. The formal solution to Eq. (4.13) is given by

$$x(t) = e^{tF}x(0) + \int_0^t e^{(t-s)F}\Sigma\, dw(t), \tag{4.14}$$

where $e^{tF} = \sum_{n=0}^{\infty}\frac{t^n}{n!}F^n$ is the fundamental solution to $\dot{X}(t) = FX(t)$ with $X(0) = I$, and $w(t)$ is the standard d-dimensional Wiener process. From the properties of stochastic integrals it follows that

$$\eta(t) = \int_0^t e^{(t-s)F}\Sigma\, dw(t)$$

has mean 0 and covariance

$$R(t) = E\eta(t)\eta(t)^T = \int_0^t e^{sF}\Sigma\Sigma^T e^{sF^T}\,ds, \tag{4.15}$$

where F^T is the transpose of the matrix F. The matrix $R(t)$ is nonnegative definite but not necessarily positive definite. We follow the presentation of Refs. 32 and 33. For each $t > 0$ the matrix $R(t)$ has constant rank equal to the dimension of the space

$$[F, \Sigma] := \{F^{l-1}\Sigma\epsilon_j : l, j = 1, \ldots, d, \epsilon_j = (\delta_{j1}, \ldots, \delta_{jp})^T\}.$$

If $l = \text{rank}\, R(t)$ then $d - l$ coordinates of the process $\eta(t)$ are equal to 0 and the remaining l coordinates constitute an l-dimensional Gaussian process. Thus if $l < d$ there is no stationary density. If rank $R(t) = d$ then the transition probability function of $x(t)$ is given by the Gaussian density

$$k(t, x, x_0) = \frac{\exp\left\{ -\frac{1}{2}(x - e^{tF}x_0)^T R(t)^{-1}(x - e^{tF}x_0)\right\}}{\sqrt{(2\pi)^d \det R(t)}}, \tag{4.16}$$

where $R(t)^{-1}$ is the inverse matrix of $R(t)$. An invariant density f_* exists if and only if all eigenvalues of F have negative real parts, and in this case the unique stationary density f_* has the form

$$f_*(x) = \frac{1}{\sqrt{(2\pi)^d \det R_*}} \exp\left\{-\frac{1}{2}x^T R_*^{-1} x\right\}, \tag{4.17}$$

where R_* is a positive definite matrix given by

$$R_* = \int_0^\infty e^{sF}\Sigma\Sigma^T e^{sF^T}\,ds,$$

and is a unique symmetric matrix satisfying

$$FR_* + R_*F^T = -\Sigma\Sigma^T. \tag{4.18}$$

We conclude that if $[F, \Sigma]$ contains d linearly independent vectors and all eigenvalues of F have negative real parts, then the corresponding semigroup of Markov operators is asymptotically stable. From Theorem 3 it follows that

$$\lim_{t\to\infty} H_c(P^t f_0 | f_*) = 0$$

and from Theorem 4 that

$$\lim_{t\to\infty} H_G(P^t f_0) = H_G(f_*)$$

for all f_0 with $H_c(f_0|f_*) > -\infty$.

Now let f_0 be a Gaussian density of the form

$$f_0(x) = \frac{1}{\sqrt{(2\pi)^d \det Q_0}} \exp\left\{-\frac{1}{2}x^T Q_0^{-1} x\right\}, \tag{4.19}$$

where Q_0 is a positive definite symmetric matrix. From Eq. (4.14) it follows that $x(t)$ is Gaussian with zeroth mean vector and the following covariance matrix

$$Q(t) = e^{tF} Q_0 e^{tF^T} + R(t). \tag{4.20}$$

Hence the density of $x(t)$ is given by

$$P^t f_0(x) = \frac{1}{\sqrt{(2\pi)^d \det Q(t)}} \exp\left\{-\frac{1}{2}x^T Q(t)^{-1} x\right\}. \tag{4.21}$$

Since $\int P^t f_0(x) x^T Q(t)^{-1} x \, dx = d$, the Gibbs' entropy of $P^t f_0$ is

$$H_G(P^t f_0) = \frac{1}{2}\log(2\pi)^d \det Q(t) + \frac{d}{2}. \tag{4.22}$$

By Eq. (3.1) and the formula

$$\int P^t f_0(x) x^T R_*^{-1} x \, dx = \mathrm{Tr}\,(R_*^{-1} Q(t))$$

we obtain the conditional entropy

$$\begin{aligned} H_c(P^t f_0 | f_*) = H_G(P^t f_0) - \frac{1}{2}\log(2\pi)^d \det R_* \\ -\frac{1}{2}\mathrm{Tr}\,(R_*^{-1} Q(t)) \end{aligned} \tag{4.23}$$

for all $t \geq 0$ and every f_0 of the form given by Eq. (4.19). Formula 4.22 remains valid when we start with a Gaussian density f_0 with non zero mean but then in the formula for the conditional entropy one additional term appears, see [27, Sec. 4].

Example 2. Noisy harmonic oscillator.

Consider the second order system

$$m\frac{d^2y}{dt^2} + \gamma\frac{dy}{dt} + \omega^2 y = \sigma\xi \tag{4.24}$$

with constant positive coefficients m, γ and σ. Introduce the velocity $v = \frac{dy}{dt}$ as a new variable. Then Eq. (4.24) is equivalent to the system

$$\frac{dy}{dt} = v \tag{4.25a}$$

$$m\frac{dv}{dt} = -\gamma v - \omega^2 y + \sigma\xi, \tag{4.25b}$$

and the corresponding Fokker-Planck equation is

$$\frac{\partial f}{\partial t} = -\frac{\partial [vf]}{\partial y} + \frac{1}{m}\frac{\partial [(\gamma v + \omega^2 y)f]}{\partial v} + \frac{\sigma^2}{2m^2}\frac{\partial^2 f}{\partial v^2}.$$

We can assume in what follows that $m = 1$, as introducing the constants $\tilde{\gamma} = \gamma/m$, $\tilde{\omega}^2 = \omega^2/m$ and $\tilde{\sigma}^2 = \sigma^2/m^2$ leads to

$$\frac{\partial f}{\partial t} = -\frac{\partial [vf]}{\partial y} + \frac{\partial [(\tilde{\gamma} v + \tilde{\omega}^2 y)f]}{\partial v} + \frac{\tilde{\sigma}^2}{2}\frac{\partial^2 f}{\partial v^2}.$$

The results of Sec. 4.2 in the two dimensional setting apply with $x = (y, v)^T$,

$$F = \begin{pmatrix} 0 & 1 \\ -\omega^2 & -\gamma \end{pmatrix}, \quad \text{and} \quad \Sigma = \begin{pmatrix} 0 & 0 \\ 0 & \sigma \end{pmatrix}.$$

Since

$$[F, \Sigma] = \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \sigma \end{pmatrix}, \sigma \begin{pmatrix} 1 \\ -\gamma \end{pmatrix} \right\},$$

the transition density function is given by Eq. (4.16). The eigenvalues of F are equal to

$$\lambda_1 = \frac{-\gamma + \sqrt{\gamma^2 - 4\omega^2}}{2}, \tag{4.26a}$$

$$\lambda_2 = \frac{-\gamma - \sqrt{\gamma^2 - 4\omega^2}}{2}, \tag{4.26b}$$

and are either negative real numbers when $\gamma^2 \geq 4\omega^2$ or complex numbers with negative real parts when $\gamma^2 < 4\omega^2$. Thus the stationary density is given by Eq. (4.17). As is easily seen R_*, being a solution to Eq. (4.18), is given by

$$R_* = \frac{\sigma^2}{2\gamma\omega^2} \begin{pmatrix} 1 & 0 \\ 0 & \omega^2 \end{pmatrix}.$$

The inverse of the matrix R_* is

$$R_*^{-1} = \frac{2\gamma}{\sigma^2} \begin{pmatrix} \omega^2 & 0 \\ 0 & 1 \end{pmatrix}$$

and the unique stationary density becomes

$$f_*(y, v) = \frac{\gamma\omega}{\pi\sigma^2} e^{-\frac{\gamma}{\sigma^2}[\omega^2 y^2 + v^2]}.$$

If the initial density f_0 is the Gaussian

$$f_0(y, v) = \frac{1}{2\pi\bar{\sigma}_1\bar{\sigma}_2} \exp\left\{-\frac{y^2}{2\bar{\sigma}_1^2} - \frac{v^2}{2\bar{\sigma}_2^2}\right\},$$

where $\bar{\sigma}_1 > 0$, $\bar{\sigma}_2 > 0$, then $P^t f_0$ is as in Eq. (4.21) with

$$Q(t) = e^{tF} Q_0 e^{tF^T} + R(t),$$

where

$$Q_0 = \begin{pmatrix} \bar{\sigma}_1^2 & 0 \\ 0 & \bar{\sigma}_2^2 \end{pmatrix} \tag{4.27}$$

and

$$R(t) = \int_0^t e^{sF} \begin{pmatrix} 0 & 0 \\ 0 & \sigma^2 \end{pmatrix} e^{sF^T} ds. \tag{4.28}$$

The formula for the covariance matrix $R(t)$ is given by Chandrasekhar [34, pp. 27–30]. The Gibbs' entropy is

$$H_G(P^t f_0) = 1 + \log(2\pi) + \frac{1}{2} \log\det Q(t) \tag{4.29}$$

and the conditional entropy is

$$H_c(P^t f_0|f_*) = 1 + \frac{1}{2}\log\det Q(t) - \frac{1}{2}\log\det R_* - \frac{1}{2}\operatorname{Tr}(R_*^{-1} Q(t)). \tag{4.30}$$

We are going to show that the Gibbs' entropy need not be a monotonic function of time, so we need to calculate det $Q(t)$ to have the analytic formula for the Gibbs' entropy. The calculations depend on the nature of eigenvalues λ_1 and λ_2 in Eq. (4.26), so we must distinguish between three cases: (i) Overdamped: $\lambda_1, \lambda_2 \in \mathbf{R}$ with $\lambda_1 \neq \lambda_2$, (ii) Critically damped: $\lambda_1, \lambda_2 \in \mathbf{R}$ with $\lambda_1 = \lambda_2$, and (iii) Underdamped: λ_1, λ_2 are complex.

The calculations are complex. Here we only summarize the results of the complete analysis presented in the Appendix. In the summary that follows we use the notation

$$\sigma_* = \frac{\sigma^2}{2\gamma\omega^2}, \tag{4.31a}$$

$$\alpha_1 = \bar{\sigma}_1^2 - \sigma_*, \tag{4.31b}$$

$$\alpha_2 = \bar{\sigma}_2^2 - \omega^2\sigma_*. \tag{4.31c}$$

Observe that $\alpha_1\alpha_2 = \det(Q_0 - R_*)$ and $\sigma_*^2\omega^2 = \det R_*$.

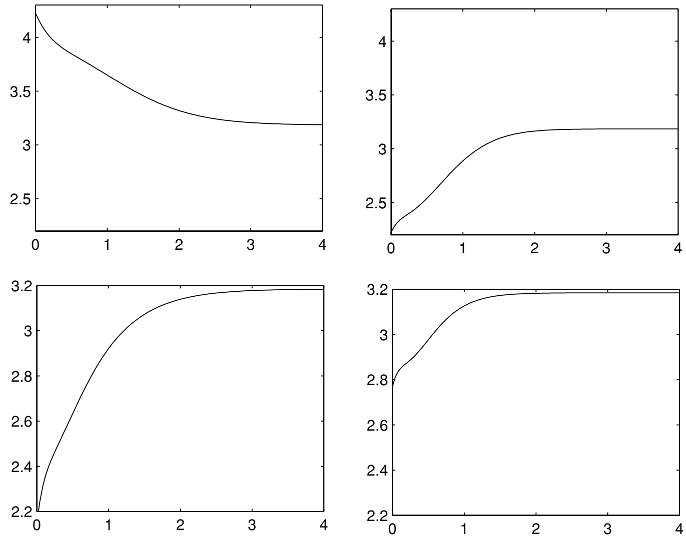

Fig. 1. Entropy behavior for the overdamped noisy harmonic oscillator when $\alpha_1\alpha_2 \geq 0$. The left hand panels show plots of $H_G(P^t f_0)$ as a function of time as given by Eq. (4.29) and the right hand panels show $H_{NE}(P^t f_0) \equiv H_c(P^t f_0|f_*) + H_G(f_*)$ as a function of time. The parameters used were $m = 1$, $\gamma = 3$, $\omega^2 = 2$, and $\sigma_* = 1$. Upper panels correspond to the range of parameters as in Eq. (A.5) with specific values $\bar{\sigma}_1 = 2$, $\bar{\sigma}_2 = 2$, while the lower panels correspond to parameters as in Eq. (A.10) with $\bar{\sigma}_1 = 0.5$, $\bar{\sigma}_2 = 1$.

The analytic results in the Appendix in the overdamped and critically damped cases indicate that there are three possible types of behaviors of the Gibbs' entropy and these are illustrated in Fig. 1 through 3. Namely, for $\alpha_1\alpha_2 \geq 0$ there can either be a monotonic decrease or increase of $H_G(P^t f_0)$ to $H_G(f_*)$ as shown in Fig. 1. For $\alpha_1\alpha_2 < 0$, $H_G(P^t f_0)$ will approach $H_G(f_*)$ through an overshoot (Fig. 2 when $\alpha_1 > 0$, $\alpha_2 < 0$) or undershoot (Fig. 3 when $\alpha_1 < 0$, $\alpha_2 > 0$). In every case the nature of the approach of $H_G(P^t f_0)$ to $H_G(f_*)$ is dependent on the variance of the initial ensemble. Also, in every case it can be shown analytically that $H_{NE}(P^t f_0) \equiv H_c(P^t f_0|f_*) + H_G(f_*)$ (c.f Sec. 5) is a smooth, monotonically increasing function that approaches $H_G(f_*)$.

In the underdamped case, the approach of $H_G(P^t f_0)$ to $H_G(f_*)$ can also be oscillatory as shown in Figs. 4 and 5 while, as expected, $H_{NE}(P^t f_0)$ monotonically increases to $H_G(f_*)$.

5. SUMMARY AND DISCUSSION

In dynamical systems (as are all fundamental descriptions in physics), the conditional entropy is constant in time and determined by the system initial

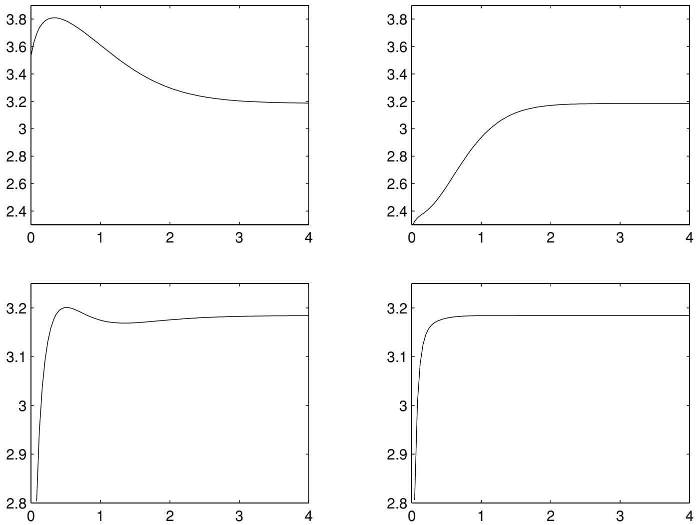

Fig. 2. Entropy behavior in the overdamped noisy harmonic oscillator with $\alpha_1 > 0, \alpha_2 < 0$. Plots and parameters as in Fig. 1, but now the upper panels are for the range of parameters as in Eq. (A.11) with $\bar{\sigma}_1 = 2, \bar{\sigma}_2 = 1$, and the lower panels as in Eq. (A.13) with $\bar{\sigma}_1 = 1.1, \bar{\sigma}_2 = 0.1$.

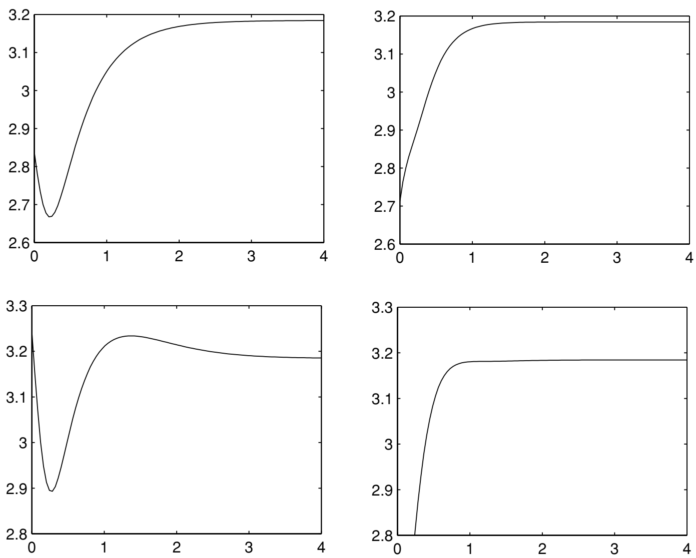

Fig. 3. Temporal behavior of the entropy in an overdamped noisy harmonic oscillator with $\alpha_1 < 0$, $\alpha_2 > 0$. Plots and paramenters as in Fig. 1, but the upper panels are for the range of parameters as in Eq. (A.15) with $\bar{\sigma}_1 = 0.5, \bar{\sigma}_2 = 2$, and the lower panels as in Eq. (A.17) $\bar{\sigma}_1 = 0.5, \bar{\sigma}_2 = 3$.

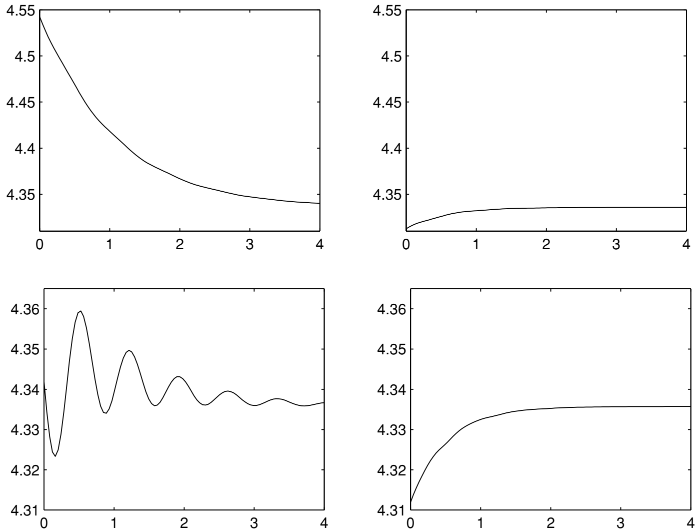

Fig. 4. The entropy behavior of an underdamped noisy harmonic oscillator as a function of time. Plots as in Fig. 1 but for parameters $\gamma = 1$, $\omega^2 = 20$, $\sigma_* = 1$. Upper panels are for the range of parameters as in Eq. (A.23) with $\bar{\sigma}_1 = 1.1$ and $\bar{\sigma}_2 = 5$, lower panels for Eq. (A.27) with $\bar{\sigma}_1 = 0.9$, $\bar{\sigma}_2 = 5$.

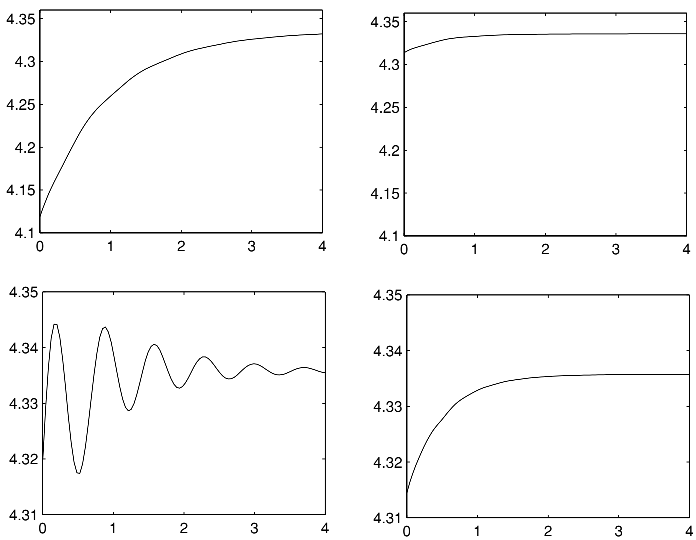

Fig. 5. Temporal entropy behavior of a underdamped noisy harmonic oscillator. Plots as in Fig. 4. Upper panels are for the range of parameters as in Eq. (A.29) with $\bar{\sigma}_1 = 0.9$ and $\bar{\sigma}_2 = 4$, lower panels for Eq. (A.30) with $\bar{\sigma}_1 = 1.1$, $\bar{\sigma}_2 = 4$.

condition (Theorem 2). Furthermore, the Gibbs' entropy of Lebesgue measure preserving dynamical systems (e.g. Hamiltonian systems) is constant.[8,10,35,36] For non-Lebesgue measure preserving dynamics, the Gibbs' entropy will increase when the dynamics are expanding and decrease if they are contracting.

To try to understand the basis for complicated and irreversible experimental observations, a number of physicists have supplemented the dynamical systems formulation of physical laws with various hypotheses about the irregularity of the physical world. One of the first of these attempts was the "molecular chaos" hypothesis of Boltzmann.[37] This hypothesis postulated a lack of correlation between the pre- and post-collision movement of molecules in a small collision volume, and allowed the derivation of the Boltzmann equation from the Liouville equation (which also led to the H theorem). In an effort to understand the nature of turbulence, Ruelle[38–40] postulated that a type of mixing dynamics was necessary. More recently, several authors have made "chaotic hypotheses" about the nature of dynamics at the microscopic level. The most prominent of these is Gallavotti,[41] and virtually the entire book of Dorfman[42] is predicated on the implicit assumption that microscopic dynamics have a chaotic (loosely defined, but usually taken to be mixing) nature.

Others have taken this chaotic hypothesis seriously and attempted an experimental confirmation. Recently Gaspard *et al.*[43] experimentally examined the trajectories of Brownian particles, and showed a positive lower bound on the sum of Lyapunov exponents of the system composed of the macroscopic Brownian particle and the surrounding fluid. They argued that the Brownian motion was due to (or the signature of) deterministic microscopic chaos. Recently, in a review Mackey and Tyran-Kamińska[46] have summarized how all of the properties of a Wiener process can be duplicated by deterministic chaotic dynamics. This suggests it is of more than passing interest to know what the effects of "noise" are on the behavior of entropy measures.

The temporal behavior of the Gibbs' entropy in systems subjected to noise can be varied. A number of authors have considered aspects of this recently, notably Ruelle,[9,10] Nicolis and Daems,[11] Daems and Nicolis,[12] Bag *et al.*,[13,14] Bag,[15–17] and Garbaczewski.[47] As we have shown in Example 1, in contrast to the conditional entropy that increases monotonically to approach zero in the presence of noise, the Gibbs' entropy can monotonically approach the equilibrium value of $H_G(f_*)$ by either increasing or decreasing and the direction of movement is totally determined by the variance $\bar{\sigma}^2$ of the initial ensemble. The temporal behavior of the Gibbs' entropy can, however, have even more complicated patterns as illustrated by Example 2.. There we have shown that when the harmonic oscillator is either over damped or critically damped, the approach of $H_G(P^t f_0)$ to $H_G(f_*)$ may be either monotonic increasing or decreasing (Fig. 1), or display either an undershoot or overshoot (Figs. 2 and 3). When the harmonic oscillator is under damped then the approach of the Gibbs' entropy to $H_G(f_*)$ may even be oscillatory as shown in Figs. 4 and 5. All of these patterns are, as we have shown, dependent on the relation of the variance of the initial ensemble to the variance of the equilibrium state. In all of these cases (over, critically, and under damped) the conditional entropy smoothly approaches zero so $H_{NE}(P^t f_0) \equiv H_c(P^t f_0|f_*) + H_G(f_*)$, as shown in the right hand panels of Fig. 1 through 5, monotonically increases to approach $H_G(f_*)$.

The Gibbs' equilibrium entropy definition Eq. (2.1) has repeatedly proven to yield correct results when applied to a variety of equilibrium situations. This is why it is the gold standard for equilibrium computations in statistical mechanics and thermodynamics. Thus it makes total sense to identify the equilibrium Gibbs' entropy $H_G(f_*)$ with the equilibrium thermodynamic entropy.

The question of how a time dependent non-equilibrium entropy should be defined has interested investigators for some time, and specifically the question of whether the Gibbs' entropy $H_G(f)$ can be extended to a time dependent situation has occupied many researchers. Various aspects of this question have been considered.[(9,10,12–17,31,49,50)] As we have demonstrated in this paper, concrete analytic examples can be constructed in which the direction of the temporal change in $H_G(f)$ depends on the initial preparation of the system and others can be constructed in which $H_G(f)$ oscillates in time.

A number of other authors, including de Groot and Mazur [51, pp. 122–129, Eq. 247], van Kampen [52, pp. 111–114 and 185], and Penrose [53, p. 213] have suggested that a time dependent entropy should be associated dynamically with

$$
\begin{aligned}
H_{NE}(f) &\equiv H_c\big(f\,|\,f_*\,e^{H_G(f_*)}\big) \\
&= H_c(f\,|\,f_*) + H_G(f_*)
\end{aligned}
\tag{5.1}
$$

as an extension of Gibbs [8, pp. 44–45 and 168] discussion of entropy. This also goes under the name of the "Gibbs' entropy postulate."[(54–59)]

Here, we have shown that $H_{NE}(f) = H_c(f\,|\,f_*) + H_G(f_*)$ has quite different temporal behavior compared to the Gibbs' entropy. This is a consequence of the behavior of $H_c(f\,|\,f_*)$ with respect to time. Namely $H_{NE}(f)$ is either constant for dynamical systems, or monotone increasing to the equilibrium value of $H_G(f_*)$ for asymptotically stable semidynamical systems induced by noise.

APPENDIX A: THE NOISY HARMONIC OSCILLATOR

In working through the details of the noisy harmonic oscillator of Example 2, we consider three separate cases.

(i) Let us first consider the *overdamped case*

$$\gamma^2 > 4\omega^2,$$

so the eigenvalues in Eq. (4.26) are real and $\lambda_1 \neq \lambda_2$. Define, for $t \geq 0$,

$$c_1(t) = \frac{\lambda_2 \, e^{\lambda_1 t} - \lambda_1 \, e^{\lambda_2 t}}{\lambda_2 - \lambda_1}, \tag{A.1a}$$

$$c_2(t) = \frac{e^{\lambda_2 t} - e^{\lambda_1 t}}{\lambda_2 - \lambda_1}. \tag{A.1b}$$

Then

$$e^{tF} = \begin{pmatrix} c_1(t) & c_2(t) \\ c_1'(t) & c_2'(t) \end{pmatrix}$$

and the covariance matrix $R(t)$ is given by

$$R(t) = R_* - \frac{\sigma^2}{2\gamma\omega^2} \begin{pmatrix} c_1^2 + \omega^2 c_2^2 & -\gamma\omega^2 c_2^2 \\ -\gamma\omega^2 c_2^2 & (c_1')^2 + \omega^2 (c_2')^2 \end{pmatrix},$$

where we suppressed the dependence of c_1 and c_2 on t. Accordingly, for Q_0 as in Eq. (4.27) we have

$$e^{tF} Q_0 \, e^{tF^T} = \begin{pmatrix} c_1^2 \bar{\sigma}_1^2 + c_2^2 \bar{\sigma}_2^2 & c_1 c_1' \bar{\sigma}_1^2 + c_2 c_2' \bar{\sigma}_2^2 \\ c_1 c_1' \bar{\sigma}_1^2 + c_2 c_2' \bar{\sigma}_2^2 & (c_1')^2 \bar{\sigma}_1^2 + (c_2')^2 \bar{\sigma}_2^2 \end{pmatrix}.$$

From Eq. (A.1) it follows that

$$c_1 c_1' + \omega^2 c_2 c_2' = -\gamma\omega^2 c_2^2.$$

Combining the three preceding equations and introducing the values of σ_*, α_1, and α_2 from Eq. (4.31), we obtain for the matrix $Q(t)$ the formula

$$Q(t) = \begin{pmatrix} c_1^2 \alpha_1 + c_2^2 \alpha_2 + \sigma_* & c_1 c_1' \alpha_1 + c_2 c_2' \alpha_2 \\ c_1 c_1' \alpha_1 + c_2 c_2' \alpha_2 & (c_1')^2 \alpha_1 + (c_2')^2 \alpha_2 + \omega^2 \sigma_* \end{pmatrix}.$$

Hence

$$\det Q(t) = \omega^2 \sigma_*^2 + \alpha_1 \alpha_2 (c_1 c_2' - c_1' c_2)^2 + \sigma_* \left(\left(\omega^2 c_1^2 + (c_1')^2\right) \alpha_1 + \left(\omega^2 c_2^2 + (c_2')^2\right) \alpha_2 \right).$$

Making use of Eq. (A.1) together with the relations $\lambda_1 \lambda_2 = \omega^2$ and $\lambda_1 + \lambda_2 = -\gamma$, we arrive at

$$\det Q(t) = \omega^2 \sigma_*^2 + \alpha_1 \alpha_2 \, e^{-2\gamma t} - \frac{\sigma_*}{(\lambda_1 - \lambda_2)^2} \left(\gamma \lambda_1 \left(\lambda_2^2 \alpha_1 + \alpha_2\right) e^{2\lambda_1 t} + 4\omega^2 (\omega^2 \alpha_1 + \alpha_2) \, e^{-\gamma t} + \gamma \lambda_2 \left(\lambda_1^2 \alpha_1 + \alpha_2\right) e^{2\lambda_2 t} \right).$$

Consequently, after some algebra we obtain

$$\frac{dH(P^t f_0)}{dt} = -\frac{\gamma\left(\alpha_1\alpha_2\, e^{-2\gamma t} + \sigma_*\left(c_2^2\omega^4\alpha_1 + (c_2')^2\alpha_2\right)\right)}{\det Q(t)} \tag{A.2}$$

and

$$\left(\frac{dH_G(P^t f_0)}{dt}\right)_{t=0} = -\frac{\gamma\alpha_2}{\bar{\sigma}_2^2}\begin{cases} < 0 & \text{for } \alpha_2 > 0, \\ > 0 & \text{for } \alpha_2 < 0. \end{cases} \tag{A.3}$$

Since $\gamma > 0$ and $\det Q(t) > 0$, the sign of the derivative of $H_G(P^t f_0)$ is completely determined by the remaining parts and depends on the sign of α_1 and α_2 and their mutual relations. In the case of $\alpha_1\alpha_2 = 0$ we conclude from Eqs. (A.2) and (4.31) that

$$\frac{dH_G(P^t f_0)}{dt}\begin{cases} = 0 & \text{for } \bar{\sigma}_1^2 = \sigma_*,\ \bar{\sigma}_2^2 = \omega^2\sigma_*, \\ > 0 & \text{for } \begin{matrix} \bar{\sigma}_1^2 = \sigma_*,\ \bar{\sigma}_2^2 < \omega^2\sigma_*, \\ \bar{\sigma}_1^2 < \sigma_*,\ \bar{\sigma}_2^2 = \omega^2\sigma_*, \end{matrix} \\ < 0 & \text{for } \begin{matrix} \bar{\sigma}_1^2 = \sigma_*,\ \bar{\sigma}_2^2 > \omega^2\sigma_*, \\ \bar{\sigma}_1^2 > \sigma_*,\ \bar{\sigma}_2^2 = \omega^2\sigma_* \end{matrix} \end{cases} \tag{A.4}$$

for all $t \geq 0$. Now assume that $\alpha_1\alpha_2 \neq 0$. It also follows directly from Eq. (A.2) that

$$\frac{dH_G(P^t f_0)}{dt} < 0 \quad \text{for } \bar{\sigma}_1^2 > \sigma_*, \bar{\sigma}_2^2 > \omega^2\sigma_*. \tag{A.5}$$

This behavior is illustrated in Fig. 1.

To study the remaining cases we rewrite Eq. (A.2) in the form

$$\frac{dH_G(P^t f_0)}{dt} = \frac{\gamma}{\det Q(t)}\, e^{-2\gamma t} h_1(t), \tag{A.6}$$

where

$$\begin{aligned} h_1(t) = {} & -\alpha_1\alpha_2 - \sigma_*(\lambda_1\beta_1\, e^{-2\lambda_2 t} + \lambda_2\beta_2\, e^{-2\lambda_1 t}) \\ & -2\sigma_*\frac{\omega^2}{\gamma}(\beta_1 + \beta_2)\, e^{-\gamma t} \end{aligned} \tag{A.7}$$

and

$$\beta_1 = \frac{\lambda_1(\lambda_2^2\alpha_1 + \alpha_2)}{(\lambda_1 - \lambda_2)^2}, \tag{A.8a}$$

$$\beta_2 = \frac{\lambda_2(\lambda_1^2\alpha_1 + \alpha_2)}{(\lambda_1 - \lambda_2)^2}. \tag{A.8b}$$

Since $\lambda_1\lambda_2 = \omega^2$, we obtain

$$h_1'(t) = 2\omega^2\sigma_*(\beta_1\, e^{-2\lambda_2 t} - (\beta_1 + \beta_2)\, e^{-\gamma t} + \beta_2\, e^{-2\lambda_1 t}),$$

which leads to

$$h_1'(t) = 2\omega^2\sigma_* \, e^{-2\lambda_1 t}\left(e^{(\lambda_1-\lambda_2)t} - 1\right)\left(\beta_1 \, e^{(\lambda_1-\lambda_2)t} - \beta_2\right).$$

For $t_* > 0$ such that $\beta_1 \, e^{(\lambda_1-\lambda_2)t_*} = \beta_2$ we have

$$h_1(t_*) = -\alpha_1\left(\alpha_2 + \omega^2\sigma_*\left(\frac{\beta_2}{\beta_1}\right)^{\gamma/(\lambda_1-\lambda_2)}\right). \tag{A.9}$$

Returning to formulae (A.8), we note that

$$\frac{\beta_2}{\beta_1} = 1 + \frac{(\lambda_1-\lambda_2)(\omega^2\alpha_1-\alpha_2)}{\lambda_1(\lambda_2^2\alpha_1+\alpha_2)}.$$

We can now continue to study the of behavior of $H_G(P^t f_0)$. First, we consider the case of $\alpha_1 < 0$ and $\alpha_2 < 0$. If $\omega^2\alpha_1 \geq \alpha_2$ then $h_1(t) \geq h_1(0)$ and $h_1(0) > 0$ by Eq. (A.3). Now if $\omega^2\alpha_1 < \alpha_2$ then $h_1(t) \geq h_1(t_*)$ and from Eq. (A.9) it follows that $h_1(t_*) > 0$. Consequently, we obtain

$$\frac{dH_G(P^t f_0)}{dt} > 0 \quad \text{for } \bar{\sigma}_1^2 < \sigma_*, \quad \bar{\sigma}_2^2 < \omega^2\sigma_*. \tag{A.10}$$

Consider now the case of $\alpha_1 > 0$ and $\alpha_2 < 0$. Then we know that $h_1(0) > 0$. Now if $\lambda_2^2\alpha_1 + \alpha_2 \geq 0$ then $\beta_1 \leq 0$ and $\beta_1 \leq \beta_2$. Thus h_1 is decreasing and diverges to $-\infty$ as $t \to \infty$. Consequently, if $\lambda_2^2\alpha_1 \geq -\alpha_2 > 0$, or equivalently

$$\lambda_2^2\bar{\sigma}_1^2 + \bar{\sigma}_2^2 + \gamma\lambda_2\sigma_* \geq 0 \quad \text{and} \quad \bar{\sigma}_2^2 < \omega^2\sigma_*, \tag{A.11}$$

then there is $t_0 > 0$ such that

$$\frac{dH_G(P^t f_0)}{dt}\begin{cases} > 0 & \text{for } t < t_0, \\ < 0 & \text{for } t > t_0. \end{cases} \tag{A.12}$$

If $\lambda_2^2\alpha_1 + \alpha_2 < 0$ then $\beta_1 > 0$ and $\beta_2/\beta_1 > 1$. From Eq. (A.9) it follows that $h_1(t_*) < 0$. Thus h_1 starting from a positive value at 0 decreases to a negative value at t_* and then increases and diverges to ∞. Hence we conclude that, if $0 < \lambda_2^2\alpha_1 < -\alpha_2$, or equivalently

$$\lambda_2^2\bar{\sigma}_1^2 + \bar{\sigma}_2^2 + \gamma\lambda_2\sigma_* < 0 \quad \text{and} \quad \bar{\sigma}_1^2 > \sigma_*, \tag{A.13}$$

then there are $t_1, t_2 > 0$ such that

$$\frac{dH_G(P^t f_0)}{dt}\begin{cases} > 0 & \text{for } 0 < t < t_1, \\ < 0 & \text{for } t_1 < t < t_2, \\ > 0 & \text{for } t > t_2. \end{cases} \tag{A.14}$$

These behaviors are illustrated in Fig. 2.

A symmetric behavior is observed when $\alpha_1 < 0$ and $\alpha_2 > 0$, and graphically shown in Fig. 3. We then have $h_1(0) < 0$ and a similar analysis leads to the following conclusions. If $\lambda_2^2\alpha_1 \le -\alpha_2 < 0$, or equivalently

$$\lambda_2^2\bar{\sigma}_1^2 + \bar{\sigma}_2^2 + \gamma\lambda_2\sigma_* \le 0 \quad \text{and} \quad \bar{\sigma}_2^2 > \omega^2\sigma_*, \tag{A.15}$$

then there is $t_0 > 0$ such that

$$\frac{dH_G(P^t f_0)}{dt} \begin{cases} < 0 & \text{for } t < t_0, \\ > 0 & \text{for } t > t_0 \end{cases} \tag{A.16}$$

and if $0 > \lambda_2^2\alpha_1 > -\alpha_2$, or equivalently

$$\lambda_2^2\bar{\sigma}_1^2 + \bar{\sigma}_2^2 + \gamma\lambda_2\sigma_* > 0 \quad \text{and} \quad \bar{\sigma}_1^2 < \sigma_*, \tag{A.17}$$

then there are $t_1, t_2 > 0$ such that

$$\frac{dH_G(P^t f_0)}{dt} \begin{cases} < 0 & \text{for } 0 < t < t_1, \\ > 0 & \text{for } t_1 < t < t_2, \\ < 0 & \text{for } t > t_2. \end{cases} \tag{A.18}$$

(ii) Let us now consider the *critical damping* situation when

$$\gamma^2 = 4\omega^2,$$

so that $\lambda_1 = \lambda_2$, and set

$$\lambda = -\frac{\gamma}{2}.$$

In this case we have

$$F = \begin{pmatrix} 0 & 1 \\ -\lambda^2 & 2\lambda \end{pmatrix} \quad \text{and} \quad e^{tF} = e^{\lambda t}\begin{pmatrix} 1-\lambda t & t \\ -\lambda^2 t & 1+\lambda t \end{pmatrix},$$

so that the corresponding covariance matrix $R(t)$ is given by

$$R(t) = R_* + \frac{\sigma^2 e^{2\lambda t}}{4\lambda^3}\begin{pmatrix} (1-\lambda t)^2 + \lambda^2 t^2 & 2\lambda^3 t^2 \\ 2\lambda^3 t^2 & (\lambda + \lambda^2 t)^2 + \lambda^4 t^2 \end{pmatrix}.$$

We also have

$$e^{tF} Q_0 e^{tF^T} = e^{2\lambda t}\begin{pmatrix} \bar{\sigma}_1^2(1-\lambda t)^2 + \bar{\sigma}_2^2 t^2 & -\bar{\sigma}_1^2\lambda^2 t(1-\lambda t) + \sigma_2^2 t(1+\lambda t) \\ -\bar{\sigma}_1^2\lambda^2 t(1-\lambda t) + \sigma_2^2 t(1+\lambda t) & \bar{\sigma}_1^2\lambda^4 t^2 + \bar{\sigma}_2^2(1+\lambda t)^2 \end{pmatrix}.$$

Note that now $\sigma_* = -\frac{\sigma^2}{4\lambda^3}$ and $\omega^2 = \lambda^2$. Thus

$$Q(t) = \begin{pmatrix} e^{2\lambda t}(\alpha_1(1-\lambda t)^2 + \alpha_2 t^2) + \sigma_* & e^{2\lambda t}(-\lambda^2 t^2(1-\lambda t)\alpha_1 + t(1+\lambda t)\alpha_2) \\ e^{2\lambda t}(-\lambda^2 t^2(1-\lambda t)\alpha_1 + t(1+\lambda t)\alpha_2) & e^{2\lambda t}(\alpha_1\lambda^4 t^2 + \alpha_2(1+\lambda t)^2) + \lambda^2\sigma_* \end{pmatrix},$$

where α_1 and α_2 are given by Eq. (4.31). Hence

$$\det Q(t) = \lambda^2\sigma_*^2 + \alpha_1\alpha_2\, e^{4\lambda t} + \sigma_*\, e^{2\lambda t}(\alpha_1\lambda^2((1-\lambda t)^2 + \lambda^2 t^2) + \alpha_2((1+\lambda t)^2 + \lambda^2 t^2)),$$

and after some algebra we obtain

$$\frac{dH_G(P^t f_0)}{dt} = \frac{2\lambda}{\det Q(t)}\, e^{4\lambda t}(\alpha_1\alpha_2 + \sigma_*\alpha_1\lambda^4 t^2\, e^{-2\lambda t} + \sigma_*\alpha_2(1+\lambda t)^2\, e^{-2\lambda t}). \tag{A.19}$$

Since $\lambda = -\gamma/2$, Eq. (A.3) remains valid. Now the analysis and conclusions are similar to the overdamped case. First, observe that from Eq. (A.19) follow Eq. (A.4) in the case of $\alpha_1\alpha_2 = 0$ and Eq. (A.5) in the case of positive α_1 and α_2, so assume that $\alpha_1\alpha_2 \neq 0$. Let us rewrite Eq. (A.19) in the form

$$\frac{dH_G(P^t f_0)}{dt} = \frac{\gamma}{\det Q(t)}\, e^{-2\gamma t} h_2(t),$$

where now

$$h_2(t) = -\alpha_1\alpha_2 - \sigma_*\, e^{-2\lambda t}(\alpha_1\lambda^4 t^2 + \alpha_2(1+\lambda t)^2).$$

Then

$$h_2'(t) = 2\lambda^2\sigma_*\, e^{-2\lambda t} t(\lambda(\lambda^2\alpha_1 + \alpha_2)t - (\lambda^2\alpha_1 - \alpha_2)).$$

Note that for

$$t_* = \frac{\lambda^2\alpha_1 - \alpha_2}{\lambda(\lambda^2\alpha_1 + \alpha_2)}$$

we have

$$h_2(t_*) = -\alpha_1(\alpha_2 + \lambda^2\sigma_*\, e^{-2\lambda t_*}).$$

A similar analysis as in the overdamped case leads to the same conclusions so that Eq. (A.10) remains valid in the case of negative α_1 and α_2 and also Eqs. (A.12)–(A.18) hold in the same ranges of parameters in the case of $\alpha_1\alpha_2 < 0$.

(iii) Finally, let us consider the *underdamped* case

$$\gamma^2 < 4\omega^2,$$

so that λ_1, λ_2 are complex, and set

$$\lambda = -\frac{\gamma}{2} \quad \text{and} \quad \beta = \sqrt{\omega^2 - \lambda^2}.$$

Then $\lambda_1 = \lambda + i\beta$ and $\lambda_2 = \lambda - i\beta$. The fundamental matrix in this case is equal to

$$e^{tF} = \frac{e^{\lambda t}}{\beta}\begin{pmatrix} \beta\cos(\beta t) - \lambda\sin(\beta t) & \sin(\beta t) \\ -\omega^2\sin(\beta t) & \beta\cos(\beta t) + \lambda\sin(\beta t), \end{pmatrix}.$$

Let us rewrite the matrix e^{tF} as

$$e^{tF} = \frac{e^{\lambda t}}{\beta}\begin{pmatrix} c_3(t) & \sin(\beta t) \\ -\omega^2\sin(\beta t) & c_4(t) \end{pmatrix},$$

where

$$c_3(t) = \beta\cos(\beta t) - \lambda\sin(\beta t), \tag{A.20a}$$

$$c_4(t) = \beta\cos(\beta t) + \lambda\sin(\beta t). \tag{A.20b}$$

Observe that σ_* as defined in Eq. (4.31a) is equal to $-\sigma^2/4\lambda\omega^2$. The covariance matrix $R(t)$ is equal to

$$R_* - \frac{\sigma_*\, e^{2\lambda t}}{\beta^2}\begin{pmatrix} c_3^2(t) + \omega^2\sin^2(\beta t) & 2\lambda\omega^2\sin^2(\beta t) \\ 2\lambda\omega^2\sin^2(\beta t) & \omega^4\sin^2(\beta t) + \omega^2 c_4^2(t) \end{pmatrix}.$$

Further

$$e^{tF}\begin{pmatrix} \bar{\sigma}_1^2 & 0 \\ 0 & \bar{\sigma}_2^2 \end{pmatrix} e^{tF^T}$$
$$= \frac{e^{2\lambda t}}{\beta^2}\begin{pmatrix} \bar{\sigma}_1^2 c_3^2(t) + \bar{\sigma}_2^2\sin^2(\beta t) & \left(-\omega^2\bar{\sigma}_1^2 c_3(t) + \bar{\sigma}_2^2 c_4(t)\right)\sin(\beta t) \\ \left(-\omega^2\bar{\sigma}_1^2 c_3(t) + \bar{\sigma}_2^2 c_4(t)\right)\sin(\beta t) & \omega^4\bar{\sigma}_1^2\sin^2(\beta t) + \bar{\sigma}_2^2 c_4^2(t) \end{pmatrix}.$$

Making use of expressions (4.31) and (A.20), the sum of the matrices in the two preceding equations gives

$$Q(t) = \begin{pmatrix} \sigma_* + \frac{e^{2\lambda t}}{\beta^2}\left(\alpha_1 c_3^2(t) + \alpha_2\sin^2(\beta t)\right) & \frac{e^{2\lambda t}}{\beta^2}\sin(\beta t)(\alpha_2 c_4(t) - \omega^2\alpha_1 c_3(t)) \\ \frac{e^{2\lambda t}}{\beta^2}\sin(\beta t)(\alpha_2 c_4(t) - \omega^2\alpha_1 c_3(t)) & \sigma_*\omega^2 + \frac{e^{2\lambda t}}{\beta^2}\left(\omega^4\alpha_1\sin^2(\beta t) + \alpha_2 c_4^2(t)\right) \end{pmatrix},$$

which after some algebra leads to

$$\begin{aligned} \det Q(t) = \omega^2\sigma_*^2 + e^{4\lambda t}\alpha_1\alpha_2 + \frac{\sigma_*\, e^{2\lambda t}}{\beta^2}(\omega^2(\omega^2\alpha_1 + \alpha_2) \\ -\lambda^2(\omega^2\alpha_1 + \alpha_2)\cos(2\beta t) \\ -\lambda\beta(\omega^2\alpha_1 - \alpha_2)\sin(2\beta t)). \end{aligned} \tag{A.21}$$

We have

$$\frac{dH_G(P^t f_0)}{dt} = \frac{2\lambda}{\det Q(t)} e^{2\lambda t}\biggl(\alpha_1\alpha_2\, e^{2\lambda t} + \frac{\sigma_*}{\beta^2}\left(\omega^4\alpha_1 \sin^2(\beta t) + \alpha_2 c_4^2(t)\right)\biggr). \tag{A.22}$$

Since $\lambda = -\gamma/2$, Eq. (A.3) holds. Again, Eq. (A.22) implies Eq. (A.4) in the case of $\alpha_1\alpha_2 = 0$. In the case of positive α_1 and α_2 the Gibbs' entropy is decreasing. This corresponds to

$$\bar{\sigma}_1^2 > \sigma_* \quad \text{and} \quad \bar{\sigma}_2^2 > \omega^2\sigma_*, \tag{A.23}$$

and is illustrated in Fig. 4.

Let us rewrite Eq. (A.22) in the form

$$\frac{dH_G(P^t f_0)}{dt} = \frac{\gamma}{\det Q(t)}\, e^{4\lambda t} h_3(t),$$

where now

$$h_3(t) = -\alpha_1\alpha_2 - \frac{\sigma_*}{\beta^2}\, e^{-2\lambda t}\left(\omega^4\alpha_1 \sin^2(\beta t) + \alpha_2 c_4^2(t)\right).$$

We have

$$h_3'(t) = \frac{2\omega^2\sigma_*}{\beta^2}\, e^{-2\lambda t} \sin(\beta t)(\lambda(\omega^2\alpha_1 + \alpha_2)\sin(\beta t) + \beta(\alpha_2 - \omega^2\alpha_1)\cos(\beta t)).$$

The function h_3 has extreme values at all t for which either $\sin(\beta t) = 0$ or

$$\beta\cos(\beta t) = \lambda \sin(\beta t)\frac{(\omega^2\alpha_1 + \alpha_2)}{(\omega^2\alpha_1 - \alpha_2)}. \tag{A.24}$$

Making use of the relations $\omega^2 = \lambda^2 + \beta^2$ and $\lambda = -\gamma/2$ it is seen that for every nonnegative integer k we have

$$h_3(k\pi/\beta) = -\alpha_2(\alpha_1 + \sigma_*\, e^{\gamma k\pi/\beta}) \tag{A.25}$$

and

$$h_3(t_* + k\pi/\beta) = -\alpha_1\left(\alpha_2 + \sigma_*\omega^2\, e^{\gamma(t_* + k\pi/\beta)}\right), \tag{A.26}$$

where t_* is the smallest positive solution of Eq. (A.24). Thus, if $\alpha_1 < 0$ and $\alpha_2 > 0$ then $h_3(k\pi/\beta) < 0$ and $h_3(t_* + k\pi/\beta) > 0$ for all k. Consequently, if

$$\bar{\sigma}_1^2 < \sigma_* \quad \text{and} \quad \bar{\sigma}_2^2 > \omega^2\sigma_*, \tag{A.27}$$

then there are two infinite sequences of points t_k and $\bar{t}_k$ such that

$$\frac{dH_G(P^t f_0)}{dt} \begin{cases} < 0 & \text{for } t_k < t < \bar{t}_k, \\ > 0 & \text{for } \bar{t}_k < t < t_{k+1}. \end{cases} \tag{A.28}$$

Consider now the case of $\alpha_2 < 0$. From Eq. (A.25) it follows that $h_3(k\pi/\beta) > 0$. When $\alpha_1 < 0$ the values of h_3 at $t_* + k\pi/\beta$ are positive. Therefore $h_3(t) > 0$ for all $t > 0$. Consequently, if

$$\bar{\sigma}_1^2 < \sigma_* \quad \text{and} \quad \bar{\sigma}_2^2 < \omega^2 \sigma_*, \tag{A.29}$$

then the Gibbs' entropy increases. Finally, when $\alpha_1 > 0$ then $\alpha_2 < \omega^2 \alpha_1$, the function h_3 decreases from a positive value at $k\pi/\beta$ to a negative value at $t_* + k\pi/\beta$ and then increases back to a positive value. Thus, if

$$\bar{\sigma}_1^2 > \sigma_* \quad \text{and} \quad \bar{\sigma}_2^2 < \omega^2 \sigma_*, \tag{A.30}$$

then there are two infinite sequences of points t_k and $\bar{t}_k$ such that

$$\frac{dH_G(P^t f_0)}{dt} \begin{cases} > 0 & \text{for } t_k < t < \bar{t}_k, \\ < 0 & \text{for } \bar{t}_k < t < t_{k+1}. \end{cases} \tag{A.31}$$

These behaviors are illustrated in Fig. 5.

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REFERENCES

1. K. Loskot and R. Rudnicki, *Ann. Pol. Math.* **52**: 140 (1991).
2. A. Abbondandolo, *Stoch. Anal. Applic.* **17**: 131 (1999).
3. G. Toscani and C. Villani, *J. Stat. Phys.* **98**: 1279 (2000).
4. A. Arnold, P. Markowich, G. Toscani and A. Unterreiter, *Comm. Partial Differential Equations* **26**: 43 (2001).
5. H. Qian, *Phys. Rev. E* **63**: 042103 (2001).
6. H. Qian, M. Qian and X. Tang, *J. Stat. Phys.* **107**: 1129 (2002).
7. P. Markowich and C. Villani, *Mat. Contemp.* **19**: 1 (2000).
8. J. Gibbs, *Elementary Principles in Statistical Mechanics* (Dover, New York, 1962).
9. D. Ruelle, *J. Stat. Phys.* **85**: 1 (1996).
10. D. Ruelle, *Proc. Nat. Acad. Sci.* **100**: 3054 (2003).
11. G. Nicolis and D. Daems, *Chaos* **8**: 311 (1998).
12. D. Daems and G. Nicolis, *Phys. Rev. E* **59**: 4000 (1999).
13. B. Bag, J. Chaudhuri and D. Ray, *J. Phys. A* **33**: 8331 (2000).
14. B. Bag, S. Banik and D. Ray, *Phys. Rev. E* **64**: 026110 (2001).

15. B. Bag, *Phys. Rev. E* **66**: 026122 (2002).
16. B. Bag, *Phys. Rev. E* **65**: 046118 (2002).
17. B. Bag, *J. Chem. Phys.* **119**: 4988 (2003).
18. A. Khinchin, *Mathematical Foundations of Statistical Mechanics* (Dover, New York, 1949).
19. B. Skagerstam, *Z. Naturforsch.* **29A**: 1239 (1974).
20. A. Lasota and M. C. Mackey, *Chaos, Fractals and Noise: Stochastic Aspects of Dynamics* (Springer-Verlag, Berlin, New York, Heidelberg, 1994).
21. B. C. Eu, *J. Chem. Phys.* **102** (1995).
22. B. C. Eu, *J. Chem. Phys.* **106** (1997).
23. M. Q. D-q Jian and M. p Qian, *Commun. Math. Phys.* **214** (2000).
24. H. Qian, *J. Phys. Chem.* **106**: 2065 (2002).
25. M. C. Mackey, *Time's Arrow: The Origins of Thermodynamic Behaviour* (Springer-Verlag, Berlin, New York, Heidelberg, 1992).
26. J. Voigt, *Commun. Math. Phys.* **81**: 31 (1981).
27. M. C. Mackey and M. Tyran-Kamińska, *Physica A* **365**: 360 (2006).
28. I. Csiszár, *Ann. Probability* **3**: 146 (1975).
29. W. Horsthemke and R. Lefever, *Noise Induced Transitions: Theory and Applications in Physics, Chemistry and Biology* (Springer-Verlag, Berlin, New York, Heidelberg, 1984).
30. H. Risken, *The Fokker-Planck Equation* (Springer-Verlag, Berlin, New York, Heidelberg, 1984).
31. P. Majee and B. Bag, *J. Phys. A* **37**: 3353 (2004).
32. M. Zakai and J. Snyders, *J. Differential Equations* **8**: 27 (1970).
33. R.V. Erickson, *Ann. Math. Statist.* **42**: 820 (1971).
34. S. Chandrasekhar, *Rev. Mod. Phys.* **15**: 1 (1943).
35. W.-H. Steeb, *Physica A* **95**: 181 (1979).
36. L. Andrey, *Phys. Lett. A* **111**: 45 (1985).
37. L. Boltzmann, *Lectures on Gas Theory* (Dover, Mineola, N.Y., 1995).
38. D. Ruelle, *Ann. N.Y. Acad. Sci.* **316**: 408 (1978).
39. D. Ruelle, *Phys. Let.* **72A**: 81 (1979).
40. D. Ruelle, *Ann. N.Y. Acad. Sci.* **357**: 1 (1980).
41. G. Gallavotti, *Statistical Mechanics: A Short Treatise* (Springer Verlag, Berlin, New York, 1999).
42. J. Dorfman, *An Introduction to Chaos in Nonequilibrium Statistical Mechanics, vol. 14 of Cambridge Lecture Notes in Physics* (Cambridge University Press, Cambridge, New York, 1999).
43. P. Gaspard, M. Briggs, M. Francis, J. Sengers, R. Gammon, J. Dorfman and R. Calabrese, *Nature* **394**: 865 (1998).
44. M. C. Mackey, *Rev. Mod. Phys.* **61**: 981 (1989).
45. L.S. Schulman, *Time's Arrows and Quantum Measurement* (Cambridge University Press, Cambridge, 1997).
46. M.C. Mackey and M. Tyran-Kamińska, *Phys. Rep.* **422**, 167 (2006).
47. P. Garbaczewski, *Phys. Lett. A* **341**: 33 (2005).
48. L. Landau and E. Lifshitz, *Statistical Physics: Part 1*, 3rd ed. (Butterworth-Heinemann, London, 1980)
49. D. Ruelle, *Commun. Math. Phys.* **189**: 365 (1997).
50. D. Ruelle, *Phys. Today* (2004).
51. S. de Groot and P. Mazur, *Non-Equilibrium Thermodynamics* (Dover, New York, 1984).
52. N. van Kampen, *Stochastic Processes in Physics and Chemistry*, 2nd ed. (Elesvier-North Holland, Amsterdam, 1992)
53. O. Penrose, *Foundations of Statistical Mechanics*, revised ed. (Dover, Mineola, New York, 2005).
54. J. R. A. P'erez-Madrid and P. Mazur, *Physica A* **212**: 231 (1994).
55. J. Rub'i and P. Mazur, *Physica A* **250**: 253 (1998).
56. P. Mazur, *Physica A* **261**: 451 (1998).

57. J. Rub'i and P. Mazur, *Physica A* **276**: 477 (2000).
58. D. Bedeaux and P. Mazur, *Physica A* **298**: 81 (2001).
59. J. Rub'i and A. P'erez-Madrid, *Physica A* **298**: 177 (2001).