ENTROPY PRODUCTION IN NONEQUILIBRIUM STATISTICAL MECHANICS.

by David Ruelle.

Abstract. We consider systems of nonequilibrium statistical mechanics, driven by nonconservative forces and in contact with an ideal thermostat. These are smooth dynamical systems for which one can define natural stationary states μ (SRB in the simplest case) and entropy production $e(\mu)$ (minus the sum of the Lyapunov exponents in the simplest case). We give exact and explicit definitions of the entropy production $e(\mu)$ for the various situations of physical interest. We prove that $e(\mu) \geq 0$ and indicate cases where $e(\mu) > 0$. The novelty of the approach is that we do not try to compute entropy production directly, but make it depend on the identification of a natural stationary state for the system.

Memories.

My first contact with Roland L. Dobrushin consisted in the exchange of scientific papers. I did not know (or care) that he was perhaps the greatest active probabilist of the time. But I had been working on a problem of statistical mechanics with Oscar Lanford [15], and Jean Lascoux pointed out to us that Dobrushin [7], [8] had published something on the same problem. As it turned out, our results complemented his in showing that translationally invariant Gibbs states are identical with equilibrium states (in present day terminology). Then Yasha Sinai [22], [23] obtained his great results on the use of Gibbs states in hyperbolic dynamical systems, complemented later by Rufus Bowen [2]. All these results are now well known, and used without reference (as they will be in the present paper), but participating in the discovery was a great experience.

I first met Dobrushin in Moscow (the Soviet authorities did not allow him to travel to the West). He was quite outspoken about the regime, with the usual precaution of taking a little stroll in a park before saying anything compromising (not indoors!) I remember

Roland Dobrushin as smiling and fearless. When I brought him a copy of a novel by Solzhenitsyn, he thanked me by saying it was "a gift for a king", and not a word about the danger of accepting such a gift. He told me about the "extraordinary stability" of the Soviet system, expressing the belief that it would take five hundred years before it went down. There he was wrong: he lived to see the collapse of Soviet Socialism. But Nomenklaturism is not dead, and anywhere in the world we may yet have to see the people crushed in the name of the People, and freedom and democracy destroyed in the name of Freedom and Democracy. Anywhere in the world we may yet have to take a little stroll in the park to express opinions that do not conform with the official Truth.

Introduction.

A revival of nonequilibrium statistical mechanics is currently taking place, using the ideas and methods of the ergodic theory of smooth dynamical systems (see in particular Chernov et al. [4], Bunimovich and Spohn [3], Gallavotti and Cohen [11], Gallavotti [10]). In the present note we adopt this dynamical systems point of view and give (for various cases of physical interest) explicit formulae for the entropy production in terms of nonequilibrium stationary states. We check that the entropy production is nonnegative, and we sometimes can prove that it is strictly positive.

One way to approach nonequilibrium statistical mechanics is to try to define stationary states which might replace the Gibbs ensembles of equilibrium statistical mechanics. The definition of nonequilibrium stationary states of a system will involve some amount of idealization because the forces keeping the system outside of equilibrium normally produce heat, which has to be evacuated by a thermostat. We want in fact an *ideal thermostat*, such that its state is not altered by the heat it absorbs from the system.

In what follows we want to study entropy production by a system in contact with an ideal thermostat and subjected to forces that maintain it outside of equilibrium. We shall propose various expressions (depending on the type of thermostat) for *the entropy production associated with a nonequilibrium stationary state*, and show that for a *natural stationary state* the entropy production is positive.

Time evolution.

From now on we shall discretize the time, so that it takes integer values. (One may for instance consider a system with continuous time at integral multiples of some arbitrary time unit, or use a Poincaré map). Time evolution is thus given by a diffeomorphism f of a smooth compact manifold M. The so-called Gaussian thermostat (see Hoover [13]), which constrains time evolution to some *energy shell* gives just such a pair (M, f) (after discretization). The symplectic structure is lost because we use nonconservative forces. We shall need a volume element dx to define entropy, but any choice will give the same result for the entropy production. Note that the map f incorporates both the effect of the nonconservative forces and of the thermostat. Physically, f does not put energy into the system but may be thought of as pumping entropy out of it.

We now list several types of time evolutions corresponding to different ideal thermostats. (These are discussed in more details in Ruelle [20], [21]; for a physically oriented introduction to dynamical systems see Eckmann and Ruelle [9]).

(i) Diffeomorphism f of manifold M. This has been discussed above; f has an inverse f^{-1}.

(ii) Map f of M; f is not assumed to have an inverse, and the folding of M by f will contribute to entropy production. (Example: f describes a shock of a particle in a gas with the container (=thermostat) and distinct initial states may give the same final state, see Chernov and Lebowitz [6]).

(iii) Map f restricted to a neighborhood N of a compact invariant set $X \subset M$. As discussed by Gaspard and Nicolis [12], one can express diffusion coefficients in terms of the study of orbits spending a long time near X (see also [9]).

(iv) Random dynamics. Let (Ω, τ) be a dynamical system with invariant probability measure $\mathbf{P}$, and $(f_\omega)_{\omega\in\Omega}$ a family of diffeomorphisms of M. The time k map is $f_{\tau^{k-1}\omega} \circ \cdots \circ f_{\tau\omega} \circ f_\omega$ (with ω distributed according to $\mathbf{P}$). Since the action of a real thermostat is stochastic at the microscopic level, it is natural to describe it by random dynamics. A case of particular interest is when the $f_{\tau^k\omega}$ are independent. (For this case see in particular Kifer [14], Ledrappier and Young [18], Liu and Qian [19], the recent paper by Bahnmüller and Liu [1], and references quoted there).

Natural stationary states.

The dynamical systems (M, f) here considered typically only have singular invariant measures (no smooth invariant measure of the form $\underline{\rho}(x)dx$). If we start with a smooth measure $\rho(dx) = \underline{\rho}(x)dx$, apply time evolution to obtain $f^k\rho$, and let somehow $k \to \infty$, we obtain candidates for describing natural nonequilibrium states. Consider for definiteness the case (i) of a diffeomorphism f of M. Any limit ρ^* when $m \to \infty$ of

$$\frac{1}{m}\sum_{k=0}^{m-1} f^k\rho \qquad\qquad (\text{with } \rho(dx) = \underline{\rho}(x)dx)$$

is a natural nonequilibrium stationary state.

Another class of natural states are the SRB measures (named after Sinai, Ruelle, Bowen, see Ledrappier and Young [17]). The SRB states are invariant measures μ satisfying

$$h_f(\mu) = \sum \text{positive Lyapunov exponents}$$

where $h_f(\mu)$ is the *time entropy* associated with f (see [9],[17] for details).

Entropy production.

Define the entropy of a smooth probability measure $\rho(dx) = \underline{\rho}(x)dx)$ to be

$$S(\underline{\rho}) = -\int dx \underline{\rho}(x) \log \underline{\rho}(x)$$

From this, and taking limits, one obtains expressions for the entropy production per time step $e_f(\mu)$ associated with a natural stationary state μ in the above cases *(i)-(iv)*. (We shall indicate how in case *(i)*).

(i) Let $J(x)$ be the absolute value of the Jacobian of f with respect to some Riemann metric on M. If ρ has density $\underline{\rho}$ and $f\rho$ density $\underline{\rho}_1 = (\underline{\rho} \circ f^{-1})/(J \circ f^{-1})$, the entropy production is

$$e(\rho) = -[S(\underline{\rho}_1) - S(\underline{\rho})] = -\int \underline{\rho}(x)dx \log J(x) = -\int \rho(dx) \log J(x)$$

Therefore we write for a general probability measure μ

$$e_f(\mu) = -\int \mu(dx)\underline{\rho}(x) \log J(x)$$

When μ is ergodic, this is also minus the sum of all Lyapunov exponents.

(ii) We may write (disintegration of the f-invariant probability measure μ with respect to f)

$$\mu(dx) = \int \mu(dy)\nu_y(dx)$$

where ν_y is a probability measure carried by $f^{-1}\{y\}$. If ν_y has mass $c_{y\alpha}$ at x_α let $H(\nu_y) = -\sum_\alpha c_{y\alpha} \log c_{y\alpha}$ and define the *folding entropy*

$$F(\mu) = \int \mu(dy)H(\nu_y)$$

Here

$$e_f(\mu) = F(\mu) - \int \mu(dx) \log J(x)$$

(iii) In this case we use the rate of escape from X under f, which is (up to a change of sign)

$$P = \sup_\rho \{h(\rho) - \sum \text{ positive Lyapunov exponents for } (\rho, f)\} \leq 0$$

where the sup is taken over f-ergodic measures ρ with support in A. We have then the following formula for the entropy production:

$$e_{Xf}(\mu) = -P - \int \mu(dx) \log J(x)$$

The term $-P$ corresponds to a renormalization of the probability to compensate for leakage out of a neighborhood of X. In the present situation it is natural to assume that the time evolution is Hamiltonian, so that $J = 1$, and the entropy production reduces to $-P$.

(iv) A natural nonequilibrium measure is here a measure μ on $\Omega \times M$ such that its image by the projection $\Omega \times M \to \Omega$ is $\mathbf{P}$. Let J_ω denote the absolute value of the Jacobian of f_ω, then

$$e_f(\mu) = -\int \mu(d\omega dx) \log J_\omega(x)$$

Positivity of entropy production.

We consider for definiteness the case *(i)* of a diffeomorphism f of M. For every f-ergodic measure μ we have

$$h(\mu) \leq \sum \text{ positive Lyapunov exponents}$$

Replacing f by f^{-1}, this gives also

$$h(\mu) \leq -\sum \text{ negative Lyapunov exponents}$$

For a SRB state μ we have

$$h(\mu) = \sum \text{ positive Lyapunov exponents}$$

and subtracting the above inequality gives

$$0 \geq \sum \text{ all Lyapunov exponents}$$

hence $e_f(\mu) \geq 0$.

Consider now the probability measure $\rho(dx) = \underline{\rho}(x)dx$ with density $\underline{\rho}$, and assume $S(\underline{\rho})$ finite. If ρ^* is a limit of $\rho^{(m)} = (1/m)\sum_{k=0}^{m-1} \rho_k$ (with $\rho_k = f^k\rho$) we have

$$e_f(\rho^*) = \lim e_f(\rho^{(m)}) = -\lim \int dx\, \underline{\rho}^{(m)}(x) \log J(x)$$

$$= -\lim \frac{1}{m}\sum_{k=1}^{m-1} \int dx\, \underline{\rho}_k(x) \log J(x) = -\lim \frac{1}{m}\sum_{k=1}^{m-1} [S(\underline{\rho}_{k-1}) - S(\underline{\rho}_k)]$$

$$= \lim \frac{1}{m}[S(\underline{\rho}) - S(\underline{\rho}_m)]$$

which is ≥ 0 because $S(\underline{\rho}_m)$ is bounded above (by $\log \mathrm{vol} M$).

While the above arguments are very simple, the corresponding problems are more difficult in cases *(ii), (iii), (iv)* and rigorous proofs exist only under specific assumptions (for which see [20], [21]).

Strict positivity of entropy production.

When can one assert that $e_f(\mu) > 0$?

In case (i), if μ is singular with respect to the Riemann volume and has no zero Lyapunov exponent, then $e_f(\mu) > 0$. This follows from a result of Ledrappier [16], see [20].

In case (ii) note that we may have $e_f(\mu) = 0$ even if $F(\mu) > 0$. (If $f : x \mapsto 2x \pmod{1}$ and μ is Lebesgue measure, then $e_f(\mu)$ =log2-log2=0).

In case (iii) suppose that f satisfies Smale's Axiom A, and X is a basic set. The natural measure μ then satisfies

$$h(\mu) - \sum \text{positive Lyapunov exponents} = P$$

This is compatible with $e_f(\mu) = 0$ only if X is an attractor for f^{-1} and μ is the corresponding SRB measure on X (see [16]).

Finally, consider the i.i.d. subcase of case (iv), i.e., $(\Omega, \mathbf{P}) = (A^{\mathbf{Z}}, p^{\mathbf{Z}})$ and we have maps $f_\alpha : M \to M$ independently distributed according to $p(d\alpha)$. Assume furthermore that there is a steady state with density $\underline{m}$ with respect to Riemann volume. The image of $\underline{m}(x)dx$ by f_α has the density $\underline{m}_\alpha(x) = \underline{m}(f_\alpha^{-1})/J_\alpha(f_\alpha^{-1})$ and the entropy production vanishes only if $\underline{m}_\alpha(x) = \underline{m}(x)$ a.e. with respect to $p(d\alpha)\underline{m}(x)dx$. This follows from a remark by Kifer [14] (see also Ledrappier and Young [18], Ruelle [21]).

Further problems.

(a) In case *(ii)* we know that for every f-ergodic measure μ

$$h(\mu) \leq \sum \text{ positive Lyapunov exponents}$$

Under what condition is the following true?

$$h(\mu) \leq F(\mu) + \sum |\text{negative Lyapunov exponents}|$$

(The case where f is piecewise smooth and $1/J$ bounded is dealt with in [20]).

(b) The results known in case (iii) assume that f is an Axiom A diffeomorphism and X a basic set. One can prove that the natural measure μ for this case satisfies

$$h(\mu) - \sum \text{positive Lyapunov exponents} = P$$

(See [20], and also the special case treated by Chernov and Markarian [5]). There remains the problem to treat more general situations.

References.

[1] J.Bahnmüller and Liu Pei-Dong. "Characterization of measures satisfying Pesin's entropy formula for random dynamical systems." To appear.

[2] R.Bowen. *Equilibrium states and the ergodic theory of Anosov diffeomorphisms.* Lecture Notes in Math. **470**. Springer, Berlin, 1975.

[3] L.A.Bunimovich and H.Spohn. "Viscosity for a periodic two disk fluid: an existence proof." Commun. Math. Phys. **176**,661-680(1996).

[4] N.I.Chernov, G.L.Eyink, J.L.Lebowitz, and Ya.G.Sinai. "Steady-state electrical conduction in the periodic Lorentz gas." Commun. Math. Phys. **154**,569-601(1993).

[5] N.I.Chernov and R.Markarian. "Ergodic properties of Anosov maps with rectangular holes." To appear.

[6] N.I.Chernov and J.L.Lebowitz. "Stationary shear flow in boundary driven Hamiltonian systems." Phys. Rev. Letters **75**,2831-2834(1995); "Stationary nonequilibrium states in boundary driven Hamiltonian systems: shear flow." J. Statist. Phys., to appear.

[7] R.L.Dobrushin. "The description of a random field by means of conditional probabilities and conditions of its regularity." Teorija Verojatn. i Ee Prim. **13**,201-229(1968). English translation, Theory Prob. Applications **13**,197-224(1968).

[8] R.L.Dobrushin. "Gibbsian random fields for lattice systems with pairwise interactions." Funkts. Analiz i Ego Pril. **2**, No **4**,31-43(1968). English translation, Functional Anal. Appl. **2**,292-301(1968).

[9] J.-P.Eckmann and D.Ruelle. "Ergodic theory of strange attractors." Rev. Mod. Phys. **57**,617-656(1985).

[10] G.Gallavotti. "Chaotic hypothesis: Onsager reciprocity and fluctuation- dissipation theorem." J. Statist. Phys. **84**,899-926(1996).

[11] G.Gallavotti and E.G.D.Cohen. "Dynamical ensembles in nonequilibrium statistical mechanics." Phys. Rev. Letters **74**,2694-2697(1995). "Dynamical ensembles in stationary states." J. Statist. Phys. **80**,931-970(1995).

[12] P.Gaspard and G.Nicolis. "Transport properties, Lyapunov exponents, and entropy per unit time." Phys. Rev. Letters **65**,1693-1696(1990).

[13] W.G.Hoover. *Molecular dynamics.* Lecture Notes in Physics **258**. Springer, Heidelberg, 1986.

[14] Yu.Kifer. *Ergodic theory of random transformations.* Birkhäuser, Boston, 1986.

[15] O.E.Lanford and D.Ruelle. "Observables at infinity and states with short range correlations in statistical mechanics." Commun. Math. Phys. **13**,194-215(1969).

[16] F.Ledrappier. "Propriétés ergodiques des mesures de Sinai." Publ. math. IHES **59**,163-188(1984).

[17] F.Ledrappier and Young Lai-Sang. "The metric entropy of diffeomorphisms: I. Characterization of measures satisfying Pesin's formula, II. Relations between entropy, exponents and dimension." Ann. of Math. **122**,509-539,540-574(1985).

[18] F.Ledrappier and Young Lai-Sang. "Entropy formula for random transformations." Prob. Th. Rel. Fields **80**,217-240(1988).

[19] Liu Pei-Dong and Qian Min. *Smooth ergodic theory of random dynamical systems.* Lecture Notes in Mathematics **1606**. Springer, Berlin, 1995.

[20] D.Ruelle. "Positivity of entropy production in nonequilibrium statistical mechan-

ics." J. Statist. Physics **85**,1-251996).

[21] D.Ruelle. "Positivity of entropy production in the presence of a random thermostat." J. Statist. Physics, to appear.

[22] Ya.G.Sinai. "Markov partitions and C-diffeomorphisms." Funkts. Analiz i Ego Pril. **2**, No **1**,64-89(1968). English translation, Functional Anal. Appl. **2**,61-82(1968).

[23] Ya.G.Sinai. "Gibbsian measures in ergodic theory." Uspehi Mat. Nauk **27**, No **4**,21-64(1972). English translation, Russian Math. Surveys **27**, No **4**,21-69(1972).