A REMARK ON THE EQUIVALENCE OF ISOKINETIC AND ISOENERGETIC THERMOSTATS IN THE THERMODYNAMIC LIMIT.

by David Ruelle*.

Abstract. The Gaussian isokinetic and isoenergetic thermostats of Hoover and Evans are formally equivalent as remarked by Gallavotti, Rondoni and Cohen. But outside of equilibrium the fluctuations are uncontrolled and might break the equivalence. We show that equivalence is ensured if we consider an infinite system assumed to be ergodic under space translations.

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* IHES. 91440 Bures sur Yvette, France. <ruelle@ihes.fr>

1. Introduction.

In the study of nonequilibrium statistical mechanics, if nonhamiltonian forces are used to achieve nonequilibrium, a thermostat is needed to cool the system. The *Gaussian thermostats* introduced by W. Hoover and D. Evans have the great interest of respecting the deterministic character of the equations of motion (see for instance Evans and Morriss [3]). Starting with an evolution equation $\dot{x} = F(x)$ in phase space, a Gaussian thermostat constrains the evolution to a prescribed hypersurface Σ by projecting $F(x)$, for $x \in \Sigma$, to the tangent plane to Σ at x. In the present note we follow Cohen-Rondoni, and Gallavotti comparing an isokinetic and an isoenergetic thermostat, and showing that they give the same result in the limit of a large system (thermodynamic limit).

In equilibrium statistical mechanics one can show rigorously that fixing the kinetic energy is equivalent to fixing the total energy, asymptotically for large systems (see [6]). It is therefore natural to hope that something similar is true for nonequilibrium, as advocated by Gallavotti (many references, see [4], [5]) and by Cohen and Rondoni [2]. However, the entropy considerations which are available in equilibrium statistical mechanics fail utterly outside of equilibrium, *i.e.*, fluctuations of energy at fixed kinetic energy are uncontrolled, and the situation appears rather hopeless. We shall show however that the argument of Cohen and Rondoni can be modified to apply, at least formally, to the dynamics of actually infinite systems. (In a different context – at equilibrium – Sinai [7] has also shown the interest of considering the dynamics of infinite systems). Our approach will remain formal at the level of infinite system evolution equations: technical problems arise there, which do not seem directly related to the problem at hand, and are better discussed separately.

We shall consider a system of particles in d dimensions which is infinitely extended in ν dimensions, with $1 \leq \nu \leq d$, and we shall discuss states of infinitely many particles which are invariant under translations in $\mathbf{R}^\nu$. The assumption that the infinite systems dynamics is well defined, and $\mathbf{R}^\nu$-ergodicity, will be sufficient to establish the equivalence of isokinetic and isoenergetic nonequilibrium steady states

2. IK an IE dynamics.

We recall now the definition of the *Gaussian isokinetic* (IK) thermostat. We take for our configuration space M a compact subset of $\mathbf{R}^u \times \mathbf{T}^v$ where $\mathbf{T}^v$ is the v-torus, and momentum space is identified with $\mathbf{R}^{u+v}$. We assume that a force field on M is given, written as $-\text{grad}V + \xi$, where $V : M \to \mathbf{R}$ is a potential, and ξ is a nongradient vector field*. Consider now the equations of motion

$$\begin{aligned} \dot{p} &= -\partial_q V + \xi - \alpha p \\ \dot{q} &= p/m \end{aligned} \tag{1}$$

completed by elastic reflection at the boundary of M. Without the term $\xi - \alpha p$ this time evolution would be Hamiltonian. The term ξ maintains the system outside of equilibrium. The term $-\alpha p$ is the thermostat. We obtain the Gausssian isokinetic thermostat by

* Note that a change in V can be compensated by a corresponding change in ξ: the splitting of the force into two terms is arbitrary for the IK time evolution.

choosing α such that the kinetic energy is constant:

$$0 = \frac{d}{dt}\frac{p^2}{2m} = \frac{p}{m} \cdot (-\partial_q V + \xi - \alpha p)$$

i.e.,

$$\alpha = (-\partial_q V + \xi) \cdot p/p^2 \tag{2}$$

Note that if ξ is locally a gradient (corresponding to a multivalued potential function on M), the Dettmann-Morriss pairing theorem asserts that (except for one value $= 0$) the spectrum of Lyapunov exponents of an ergodic measure is symmetric with respect to some constant c which is in general nonzero. (We shall however not make use of this result).

We consider now the *Gaussian isoenergetic* (IE) thermostat associated again with the force $-\mathrm{grad}V + \xi$, but where we want to maintain fixed the energy function

$$H = p^2/2m + V(q) \tag{3}$$

The equations of motion are again of the form (1) and using (3) the isoenergetic condition is

$$0 = \dot{H} = \frac{p}{m} \cdot (-\partial_q V + \xi - \alpha p) + \partial_q V \cdot \frac{p}{m}$$

i.e.,

$$\alpha = \xi \cdot p/p^2 \tag{4}$$

With the Gaussian isoenergetic (IE) thermostat the time evolution is thus defined by (1), (4).

We consider now the IK and the IE time evolution in the infinite system limit. We want to study the time evolution of a state ρ ergodic under $\mathbf{R}^\nu$-space translations. We shall ignore existence and uniqueness problems for these evolution equations, and our discussion will thus remain formal in this respect. (In fact, the one-dimensional situation may be relatively accessible to rigorous study, but the n-dimensional case with $n \geq 2$ appears much more difficult).

Physically we may think of a system of particles in a region D invariant under $\mathbf{R}^\nu$, where $1 \leq \nu \leq \mathrm{dim}D$ but possibly $\nu < \mathrm{dim}D$. For example we may consider a shear flow between two moving plates, but we do not take the limit where these two plates are infinitely far apart, as this would introduce unwanted hydrodynamic instabilities. Another example would be a system of particles in $[0, L] \times \mathbf{R}^\nu$. In the x-direction we put an electric field and we assume a suitable boundary condition (see [1]).

The expressions $p^2 = p \cdot p$ and $\xi \cdot p$ diverge for an infinite system, but behave additively with respect to volume, and we can (under mild conditions on ρ) define the average per unit volume with respect to ρ, noted $\langle p^2 \rangle_\rho$ or $\langle \xi \cdot p \rangle_\rho$. Since ρ is ergodic, it is carried by points (in infinite phase space) for which the large volume average of p^2 or $\xi \cdot p$ is well defined and constant, equal to $\langle p^2 \rangle_\rho$ or $\langle \xi \cdot p \rangle_\rho$. The expressions V, $\partial_q V \cdot p$ behave almost additively with respect to volume and, again under mild conditions, we can define the large volume averages $\langle V\rangle_\rho$, $\langle\partial_q V\cdot p\rangle_\rho$. Again, ρ is carried by points (in infinite phase space) for which the large volume average of V or $\partial_q V\cdot p$ is well defined and constant, equal to $\langle V\rangle_\rho$ or $\langle\partial_q V\cdot p\rangle_\rho$.

In our formal treatment of the infinite system IK or IE evolution we consider the time evolution of an infinite phase space point, generic with respect to the space ergodic measure ρ, replacing the expressions (2), (4) for α by their large volume limits

$$\alpha=\langle(-\partial_q V+\xi)\cdot p\rangle_\rho/\langle p^2\rangle_\rho \tag{2'}$$

or

$$\alpha=\langle\xi\cdot p\rangle_\rho/\langle p^2\rangle_\rho \tag{4'}$$

In general ρ depends on time, and so does α given by $(2')$ or $(4')$. Suppose now that ρ is invariant under the IK or IE time evolution; then α and also V are time independent, so that

$$0=\langle\dot V\rangle_\rho=\langle\partial_q V\cdot\dot q\rangle_\rho=\frac{1}{m}\langle\partial_q V\cdot p\rangle_\rho$$

But then $(2')$ and $(4')$ coincide: the infinite system IK and IE evolutions have the same time invariant space ergodic states ρ. (Apart from the use of space ergodicity for an actually infinite system, this is the remark of Cohen and Rondoni [2]).

Note that, if we replace in (3) m by $\tilde m$ and V by $\tilde V$, imposing $\dot H=0$ yields

$$\alpha=(\frac{\tilde m}{m}\partial_q\tilde V-\partial_q V+\xi)\cdot\frac{p}{p^2}$$

and in the infinite system limit we have again equivalence with the isokinetic ensemble. On the other hand, if H is not of the form $p^2/2\tilde m+\tilde V(q)$, the Gaussian thermostat doesn't give a term of the form $-\alpha p$ in (1) and we do not have equivalence with the isokinetic ensemble in the infinite system limit.

For the purposes of nonequilibrium statistical mechanics one should presumably restrict ρ to be an infinite system SRB state (defined so that the time entropy per unit volume is equal to the sum of the positive Lyapunov exponents per unit volume). Hopefully, the space ergodic SRB states form a 2-parameter family parametrized by the average number of particles and the energy (or the kinetic energy) per unit volume. But the delicate question of identifying the natural nonequilibrium steady states is here bypassed by the remark that they are the same for the infinite system IK and IE evolutions.

In equilibrium statistical mechanics the proof of equivalence of ensembles is somewhat subtle, and uses in particular the concavity properties of the entropy (see [6]). One might think that the corresponding problem in nonequilibrium statistical mechanics would be even more difficult, and the above findings about the equivalence of IK and IE appear thus surprisingly cheap. What we have shown is however only that the IK and IE evolutions coincide (formally) in the infinite system limit; the detailed study of the natural nonequilibrium states remains to be made.

3. The constant α case.

It is of interest to consider the equations (1) with $\alpha =$ constant. For this situation one obtains the following result.

Proposition.

Consider the evolution equations

$$\dot{p} = -\partial_q V + \xi - \alpha p$$
$$\dot{q} = p/m$$

in TM, where $M \subset \mathbf{R}^u \times \mathbf{T}^v$ and we impose elastic reflection on the boundary of M. We assume that α, m are constants > 0, and that V, ξ are bounded. Then

$$\limsup_{t\to\infty}(\frac{p^2}{2m} + V) \leq \frac{\max \xi^2}{2m\alpha^2} + \max V \tag{5}$$

$$\limsup_{t\to\infty} p^2 \leq \frac{\max \xi^2}{\alpha^2} + 2m(\max V - \min V) \tag{6}$$

Furthermore, if the bounded measure ρ is invariant under time evolution and, and Φ is any continuous function we have

$$\int \rho(dp\, dq)\Phi(\frac{p^2}{2m}).(\xi \cdot p - \alpha p^2) = 0 \tag{7}$$

From the evolution equations we obtain

$$\frac{d}{dt}(\frac{p^2}{2m} + V) = \frac{p}{m} \cdot \dot{p} + \partial_q \cdot \dot{q} = \frac{p}{m} \cdot (-\partial_q V + \xi - \alpha p) + \partial_q \cdot \frac{p}{m} = \frac{p}{m} \cdot (\xi - \alpha p) \tag{8}$$

Let now $\epsilon > 0$ and suppose that

$$\frac{p^2}{2m} + V \geq \frac{\max \xi^2}{2m\alpha^2} + \max V + \epsilon \tag{9}$$

then

$$p^2 \geq \max \xi^2/\alpha^2 + \epsilon$$

or

$$\alpha|p| \geq \max|\xi| + \epsilon'$$

with $\epsilon' > 0$ and thus, in view of (8),

$$\frac{d}{dt}(\frac{p^2}{2m} + V) \leq \frac{1}{m}(|p||\xi| - \alpha|p|^2) \leq -\frac{|p|}{m}\epsilon'$$

Therefore, as long as (9) holds, we have

$$\frac{d}{dt}(\frac{p^2}{2m}+V)\le -\delta$$

for some $\delta > 0$, proving (5). From (5) we obtain immediately (6).

Let $\Psi' = \Phi$ then, by the ergodic theorem,

$$\int \rho(dp\,dq)\Phi(\frac{p^2}{2m}).(\xi\cdot p-\alpha p^2)=\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\,\Phi(\frac{p^2}{2m}).(\xi\cdot p-\alpha p^2)$$

$$=\lim_{T\to\infty}\frac{m}{T}\int_0^T dt\,\Psi'(\frac{p^2}{2m}).\frac{d}{dt}(\frac{p^2}{2m}+V)=\lim_{T\to\infty}\frac{m}{T}\int_0^T dt\,\frac{d}{dt}\Psi(\frac{p^2}{2m}+V)$$

$$=\lim_{T\to\infty}\frac{m}{T}[\Psi(\frac{p^2}{2m}+V)]_0^\infty=0$$

because Ψ is bounded in view of (5). This proves (7). $\square$

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