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H-Theorems from Macroscopic Autonomous Equations

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The H-theorem is an extension of the Second Law to a time-sequence of states that need not be equilibrium ones. In this paper we review and we rigourously establish the connection with macroscopic autonomy.

If for a Hamiltonian dynamics for many particles, the macrostate evolves autonomously, then its entropy is non-decreasing as a consequence of Liouville's theorem. That observation, made since long, is here rigorously analyzed with special care to reconcile the application of Liouville's theorem (for a finite number of particles) with the condition of autonomous macroscopic evolution (sharp only in the limit of infinite scale separation); and to evaluate the presumed necessity of a semigroup property for the macroscopic evolution.

KEY WORDS: H-theorem, entropy, irreversible equations.

1. INTRODUCTION

The point of the present paper is to make mathematically precise the application of Liouville's theorem in microscopic versions or derivations of the Second Law, under the assumption that an autonomous evolution is verified for the macroscopic variables in question. Microscopic versions of the Second Law, or perhaps more correctly, generalizations of the Second Law to nonequilibrium situations, are here referred to as H-Theorems.

The stability of points of a dynamical system can be demonstrated with the help of Lyapunov functions. Yet in general these functions are hard to find—there does not exist a construction or a general algorithm to obtain them. On the other hand, when the differential equation has a natural interpretation, as with a specific

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physical origin, we can hope to improve on trial and error. Think of the equations of irreversible thermodynamics where some approach to equilibrium is visible or at least expected. Take for example the diffusion equation

$$\frac{\partial n_t(r)}{\partial t} + \nabla \cdot J_r(n_t) = 0 \tag{1.1}$$

for the particle density $n_t(r)$ at time t and at location r in some closed box. That conservation equation is determined by the current J_r depending on the particle density via the usual phenomenology

$$\begin{aligned} J_r(n_t) &= \frac{1}{2}\chi(n_t(r))\nabla s'(n_t(r)) \\ &= -\frac{1}{2}D(n_t(r))\nabla n_t(r) \end{aligned}$$

Here $D(n_t(r))$ is the diffusion matrix, connected with the mobility matrix χ via

$$\chi(n_t(r))^{-1}D(n_t(r)) = -s''(n_t(r))\,\mathrm{Id}$$

for the identity matrix Id and the local thermodynamic entropy s. From irreversible thermodynamics the entropy should be monotone and indeed it is easy to check that $\int dr\ s(n_t(r))$ is non-decreasing in time t along (1.1).

Such equations and the identifications of monotone quantities are of course very important in relaxation problems. A generic relaxation equation is that of Ginzburg-Landau. There an order parameter m is carried to its equilibrium value via

$$\frac{dm}{dt} = -D\frac{\delta\Phi}{\delta m}$$

where D is some positive-definite operator, implying

$$\frac{d\Phi}{dt} \leq 0$$

for $\Phi(m)$ for example the Helmholtz free energy.
That scenario can be generalized. We are given a first order equation of the form

$$\frac{dm_t}{dt} = F(m_t), \quad m_t \in \mathbb{R}^\nu \tag{1.2}$$

with solution $m_t = \phi_t(m)$. Yet it is helpful to imagine extra "microscopic" structure. One supposes that (1.2) results from a law of large numbers in which m_t is the macroscopic value at time t and ϕ_t gives its autonomous evolution. At the same time, there is an entropy $H(m_t)$ associated to the macroscopic variable and

one hopes to prove that $H(m_t) \geq H(m_s)$ for $t \geq s$. That will be explained and mathematically detailed starting with Sec. 3.

Usually however, from the point of view of statistical mechanics, the problem is posed in the opposite sense. Here one looks for microscopic versions and derivations of the Second Law of thermodynamics. One starts from a microscopic dynamics and one attempts to identify a real quantity that increases along a large fraction of trajectories. We will show that such an H-theorem is valid for the Boltzmann entropy when it is defined in terms of these macroscopic observables that satisfy an autonomous equation (Propositions 3.1 and 3.2). In that context, we also discuss the role of the semigroup property of the macroscopic evolution, the influence of reversibility in the microscopic dynamics and the relation with conditions of propagation of constrained equilibrium. These results are to be considered as mathematical precisions of what has been known by many for a long time. In particular, our motivation does not come from something physically problematic in the derivation of the Second Law. The main consideration in problems of relaxation to equilibrium is the enormous scale separation between the microscopic and the macroscopic worlds: the volume in phase space that corresponds to the equilibrium values of the macroscopic quantities is so very much larger than the volume of nonequilibrium parts. A thermodynamic entropy difference $s' - s$ per particle of the order of Boltzmann's constant k_B is physically reasonable and corresponds to a total reversible heat exchange $T(S' - S) = NT(s' - s)$ of about 0.5 Joule at room temperature T and to a phase volume ratio of

$$\frac{W}{W'} = \exp -(S' - S)/k_B = e^{-10^{20}}$$

when the number of particles $N = 10^{20}$.

2. HEURISTICS OF AN H-THEOREM AND MAIN QUESTIONS

2.1. Heuristics

The word H-theorem originates from Boltzmann's work on the Boltzmann equation and the identification of the so called H-functional. The latter plays the role of entropy for a dilute gas and is monotone along the solution of the Boltzmann equation. One often does not distinguish between the Second Law and the H-theorem. Here we do (and the entropy will from now on be denoted by the symbol H).

The heuristics is simple: consider here an autonomous deterministic evolution taking macrostate M_s at time s to macrostate M_t at time $t \geq s$. Then, under the Liouville dynamics U the volume in phase space $|M_s| = |UM_s|$ is preserved. On the other hand, since about every microstate x of M_s evolves under U into one corresponding to M_t, we must have, with negligible error that $UM_s \subset M_t$. We

conclude that $|M_s| \leq |M_t|$ which gives monotonicity of the Boltzmann entropy $H = k_B \log |M|$.

That key-remark has been made before, most clearly for the first time on page 84 in Ref. 4, but see also e.g. Ref. 2 page 9–10, Ref. 3 page 280–281, Ref. 5 Fig. 1 page 47, Ref. 9 page 278, page 301, and most recently in Ref. 7, 6.

The set-up we start from in the next section is a classical dynamical system and we show in what sense one can say that when a collection of variables obtains an autonomous evolution, the corresponding entropy will be monotone. A somewhat introductory but rather formal and abstract argument goes as follows.

Consider a transformation f on states x of a measure space (Ω, ρ). The measure ρ is left invariant by f. Suppose there is a sequence $(M_n), n \in \mathbb{N}$ of subsets $M_n \subset \Omega$ for which

$$\rho((f^{-1} M_{n+1})^c \cap M_n) = 0 \tag{2.1}$$

In other words, M_{n+1} should contain about all of the image $f M_n$. Then,

$$\rho(M_{n+1}) = \rho(f^{-1} M_{n+1}) \geq \rho(f^{-1} M_{n+1} \cap M_n) = \rho(M_n)$$

and $\rho(M_n)$ or $\log \rho(M_n)$ is a non-decreasing sequence.

One can think of the M_n above as macrostates that are successively visited by the microstate in the course of time. One has in mind a partition of Ω and a map M that sends each $x \in \Omega$ to the member set of the partition to which it belongs. The partition corresponds to dividing the phase space according to the values of the relevant macroscopic variables. The entropy can be defined on microstates as

$$H(y) \equiv \log \rho(M(y)), \quad y \in \Omega$$

and if for some $x \in \Omega$ the sequence $M_n = M(f^n x)$ satisfies (2.1), then the entropy

$$H(x_n) \equiv H(f^n(x)) = \log \rho(M(f^n(x))) \tag{2.2}$$

is monotone along the path starting from x. The condition (2.1) basically requires that the transformation f gets replaced on the level of the sets M_n, i.e., on the macroscopic level, with a new autonomous dynamics.

2.2. Questions

The previous heuristics, be it verbal or in a more abstract notation, calls for some further questions and warnings. Below follows our motivation to add more mathematical precision in the next Sec. 3. The point is simply that the heuristics above cannot be taken too literally; otherwise it boils down to trivialities. The autonomy has to be relaxed to allow for nontrivial statements, and as a consequence also the semigroup structure of the macroscopic dynamics (essential for the argument and trivially true in (2.1)) might be lost in general and must be enforced.

2.2.1. Scale Separation

Remark that Liouville's theorem (or the invariance of the natural measure) is essential in the above heuristics. It employs a finite number of particles. Yet, the autonomy of the macroscopic equation is probably only satisfied in some hydrodynamic limit where also the number of particles goes to infinity. In particular, (2.1) is only expected verified in some limit where the number of degrees of freedom $N \uparrow \infty$. There is thus the question, how to mathematically formulate the conditions and conclusions in a way that is physically reasonable. In fact, if (2.1) were satisfied *exactly* for a finite system, the H-function would necessarily be constant, as we will now show.

We take the same start as above but we assume also that f is bijective and that there is a countable partition $(P_i), i \in I$ of Ω with $\rho(P_i) > 0, i \in I$, for ρ a probability measure that is left invariant by f. We assume autonomy in the sense that there is a map ϕ on I with $fP_i \subset P_{\phi i}$ up to ρ–measure zero, i.e., $\rho((f^{-1}P_{\phi i})^c \cap P_i) = 0$, cf. (2.1). We show that under these conditions the entropy is constant, i.e.,

$$\rho(P_i) = \rho(P_{\phi i}) \text{ for all } i$$

To see that, note that for all $n \in \mathbb{N}$, $\rho(P_{\phi^n i}) \geq \rho(P_i)$. Therefore, as ρ is normalized, there must be $n < m$ such that $\phi^n i = \phi^m i$. On the other hand, always ρ—measure zero, both $f\ P_{\phi^{n-1}i}$, $f\ P_{\phi^{m-1}i} \subset P_{\phi^m i} = P_{\phi^n i}$. If now $\phi^{n-1}i \neq \phi^{m-1}i$, we have the contradiction

$$\begin{aligned}\rho(P_{\phi^m i}) &\geq \rho(P_{\phi^{n-1}i}) + \rho(P_{\phi^{m-1}i}) \\ &\geq \rho(P_{\phi^{n-1}i}) + \rho(P_{\phi^n i}) = \rho(P_{\phi^{n-1}i}) + \rho(P_{\phi^m i}) \\ &> \rho(P_{\phi^m i}) \end{aligned} \tag{2.3}$$

Hence the trajectory $\phi^n i, n \in \mathbb{N}$ is a closed cycle, $\phi^k i = 1$ for some k. As a consequence, the entropy is strictly constant.

The above scenario corresponds to assuming full autonomy for the macroscopic dynamics for a finite system. As shown, then, the macroscopic dynamics cannot be irreversible. On the other hand, in a thermodynamic "infinite" system, it is typically impossible to find a partition into macrostates such that each macrostate has a non-zero measure; the equilibrium state will have full measure. Hence it is necessary to add more structure and the autonomy should only hold in a thermodynamic limit.

All that does not mean that we need to look "in the thermodynamic limit." In fact, physically speaking, we are very much interested in a statement which is true for a very large but finite number of degrees of freedom (as also stressed in Sec. 2.2.3). Such a statement will come in the Sec. 3.2.

2.2.2. Semigroup Property

Dynamical equations for macroscopic degrees of freedom have varying mathematical properties. Sometimes the macroscopic dynamics is explicitly time-dependent, such as in the case when some external force is present, and sometimes the evolution is given via a differential equation of higher order or perhaps via an integro-differential equation, containing physically important so called memory terms, or the macroscopic dynamics could very well be not deterministic at all. It is therefore appropriate to be more explicit about what we mean by autonomy and under what mathematical conditions a standard H-theorem results. The conclusion in general will be that the H-theorem with the Boltzmann entropy as presented below is verified when the autonomous equation is in a sense of first order.

To see what can happen otherwise, let us imagine that a macroscopic degree of freedom m_t in a thermodynamic system evolves according to $m_t = m_0 r^t \cos \omega t$, $|r| < 1$. An example can be found in Sec. 3.3 of Ref. 1—it is like the position of a pendulum, swinging with decreasing amplitude around its equilibrium. Obviously, if we consider m_t as the only macrovariable, then the H-function only depends on m_t and hence it cannot be monotone. Nevertheless the equation for m_t is completely determined by the value m_0 at time zero. It is only after adding other degrees of freedom, like the speed of change of the degree of freedom m_t, that we get a monotone H-function. The choice of macroscopic variables is therefore absolutely relevant. It will decide whether the macroscopic values at a later time are determined from the value of the macroscopic variables at any earlier time, as required, in (2.1). If not, one can imagine a macroscopic dynamics satisfying only

$$\rho((f^{-n} M_n)^c \cap M_0) = 0 \quad n \in \mathbb{N} \tag{2.4}$$

i.e., the initial macrostate M_0 determines the whole trajectory as well but the macrodynamics is possibly not satisfying (2.1). Loosely speaking, that can happen when almost all of a macrostate M_1 is mapped into macrostate M_2, and nearly all of M_2 is mapped into M_3, but $f\ M_1 \subset M_2$ is not typically mapped into M_3.

To get an H-theorem for the more general situation (e.g. for higher order differential equations), the entropy (2.2) would have to be generalized. In other words, condition (2.1) of autonomy goes hand in hand with the interpretation of (2.2) as an entropy.

At the other side, one wants to see whether conditions referred at as repeated randomization or molecular chaos which are indeed sometimes directly used in justifications of Markov approximations or in the derivation of autonomous macroscopic equations, are necessary for an H-theorem. Microscopically speaking, these conditions not only demand that $f\ M_n \subset M_{n+1}$, as in (2.1), but they also ask that $f\ M_n$ is so to speak randomly distributed in M_{n+1}. It is as if at every time n, the microscopic state can be thought of as randomly drawn from the set M_n. We will

show in Sec. 3.1.3 how such a type of chaoticity assumption is stronger than what we effectively mean by autonomy.

2.2.3. Corrections to the H-Theorem

For a system composed of many particles, we can expect a (first order) autonomous evolution over a certain time-scale for *a good choice* of macroscopic variables. In that case (2.2) coincides with the Boltzmann entropy: it calculates the volume in phase space compatible with some macroscopic constraint (like fixing energy and some density- or velocity profile). The identification with the thermodynamic entropy (in equilibrium) then arises from considerations of equivalence of ensembles. In a way, the H-theorem is a nonequilibrium version of the Second Law—not only considering initial and final equilibria but also the entropy of the system as it evolves possibly away from equilibrium.

Two related questions enter then. Whether one can see in what sense the H-theorem is approached as the number of degrees of freedom $N \uparrow +\infty$, and whether the corresponding "finite world" H-function can be seen to be monotone along the microscopic trajectory. The H-function then needs to be defined on the microscopic state and to be followed as the microscopic dynamics prescribes. That will be done in Sec. 3.2.

All of what follows concentrates on mathematically precise and physically reasonable formulations of (2.1) and (2.2) to obtain monotonicity of entropy. The main purpose is therefore to clarify a theoretical/mathematical question; not to include new results for specific models. The only difficulty is to identify the appropriate set of assumptions and definitions; from these the mathematical arguments will be relatively short and easy.

3. CLASSICAL DYNAMICAL SYSTEMS

Let N be an integer, to be thought of as the number of degrees of freedom or as a scaling parameter, that indexes the dynamical system $(\Omega^N, U_t^N, \rho^N)$. Ω^N is the phase space with states $x \in \Omega^N$ and is equipped with a probability measure ρ^N, invariant under the dynamics $U_t^N : \Omega^N \to \Omega^N$.

We suppose a map

$$m^N : \Omega^N \to \mathcal{F} \tag{3.1}$$

which maps every state x into an element $m^N(x)$ of a metric space $(\mathcal{F}, d)$ (independent of N). For $\mathcal{F}$ one can have in mind $\mathbb{R}^n$ for some integer n or a space of real-valued functions on a subset of $\mathbb{R}^n$, with the interpretation that $m^N(x)$ gives the macroscopic state corresponding to the microscopic state x. For $m, m' \in \mathcal{F}$ and $\delta > 0$ we introduce the notation $m' \overset{\delta}{=} m$ for $d(m', m) \leq \delta$.

3.1. Infinite Scale Separation

We start here by considering the limit $N \uparrow +\infty$. In that limit the law of large numbers starts to play with deviations governed by

$$H(m) \equiv \lim_{\delta \downarrow 0} \lim_{N \uparrow +\infty} \frac{1}{N} \log \rho^N(M^N(x) \stackrel{\delta}{=} m), \quad m \in \mathcal{F} \tag{3.2}$$

That need not exist in general, but we make that definition part of our assumptions and set-up. For what follows under Proposition 3.1 it is in fact sufficient to take the lim sup in (3.2) (if we also take the lim sup in the next (3.3)) but for simplicity we prefer here to stick to the full limit. The limit (3.2) is then a natural notion of entropy à la Boltzmann; see later in (3.15) and below for a "finite" version.

The macroscopic observables are well-chosen when they satisfy an autonomous dynamics, sharply so in the proper limit of scales. Here we assume dynamical autonomy in the following rather weak sense: there is an interval $[0, T]$ and a map $\phi_t : \mathcal{F} \to \mathcal{F}$ for all $t \in [0, T]$ such that $\forall m \in \mathcal{F}, \forall \delta > 0$, and $0 \le s \le t \le T$,

$$\lim_{\epsilon \downarrow 0} \lim_{N \uparrow +\infty} \frac{1}{N} \log \rho_N \left(m^N\left(U_t^N x\right) \stackrel{\delta}{=} \phi_t(m) | m^N\left(U_s^N x\right) \stackrel{\epsilon}{=} \phi_s(m) \right) = 0 \tag{3.3}$$

Proposition 3.1. *$\forall m \in \mathcal{F}$ and for all $0 \le s \le t \le T$,*

$$H(\phi_t(m)) \ge H(\phi_s(m)) \tag{3.4}$$

Proof: Writing out $H(\phi_t(m))$ we find that for every $\epsilon > 0$

$$\begin{aligned} \log \rho^N(m^N(x) \stackrel{\delta}{=} \phi_t(m)) &= \log \rho^N \left(m^N\left(U_t^N x\right) \stackrel{\delta}{=} \phi_t(m) \right) \\ &\ge \log \rho^N \left(m^N\left(U_t^N x\right) \stackrel{\delta}{=} \phi_t(m) | m^N\left(U_s^N x\right) \stackrel{\epsilon}{=} \phi_s(m) \right) \\ &\quad + \log \rho^N \left(m^N\left(U_t^N x\right) \stackrel{\epsilon}{=} (m) \right) \end{aligned} \tag{3.5}$$

The equality uses the invariance of ρ^N and we can use that again for the last term in (3.5). We divide (3.5) by N and we first take the limit $N \uparrow +\infty$ after which we send $\epsilon \downarrow 0$ and then $\delta \downarrow 0$. □

Condition (3.3) is much less than requiring a strict macroscopic autonomy. We do for example not suppose that the macroscopic trajectory is uniquely determined. In fact, condition (3.3) is consistent with a large class of stochastic macroscopic dynamics too.

A sufficient condition for (3.3) will follow in Sec. 3.1.3.

The case of a stochastic microscopic dynamics will be addressed in Sec. 4.

3.1.1. Semigroup Property

If the dynamics (U_t^N) satisfies the semigroup property

$$U_{t+s}^N = U_t^N U_s^N \quad t, s \geq 0 \tag{3.6}$$

and there is a unique macroscopic trajectory (ϕ_t) satisfying (3.3), then

$$\phi_{t+s} = \phi_t \circ \phi_s \quad t, s \geq 0 \tag{3.7}$$

In practice the map ϕ_t will mostly be the solution of a set of first order differential equations. Observe then that (3.7) combined with (3.3) for $s = 0$ also yields the full monotonicity (3.4).

3.1.2. Reversibility

Equation (3.3) invites the more general definition of a large deviation rate function for the transition probabilities

$$-J_{t,s}(m, m') \equiv \lim_{\delta \to 0} \lim_{\kappa \to 0} \lim_{N \to \infty} \frac{1}{N} \log \rho^N(m^N\big(U_t^N x\big) \stackrel{\delta}{=} m' | m^N\big(U_s^N x\big) \stackrel{\kappa}{=} m\big),$$
$$t \geq s \tag{3.8}$$

which we assume to exist. The bounds of (3.5) give

$$H(m') \geq H(m) - J_{t,s}(m, m') \tag{3.9}$$

for all $m, m' \in \mathcal{F}$ and $t \geq s$. In particular, quite generally,

$$H(\phi_t(m)) \leq H(\phi_s(m)) + J_{t,s}(\phi_t(m), \phi_s(m)), \quad t \geq s \tag{3.10}$$

while, as from (3.3), $J_{t,s}(\phi_s(m), \phi_t(m)) = 0$. On the other hand, if the dynamical system $(\Omega^N, U_t^N, \rho^N)$ is reversible under an involution π^N, $U_t^N = \pi^N U_{-t}^N \pi^N$ such that $\rho^N \pi^N = \rho^N$, $\pi^N m^N = m^N$, then

$$H(m') - J_{t,s}(m', m) = H(m) - J_{t,s}(m, m') \tag{3.11}$$

for all $m, m', t \geq s$. Hence, under dynamical reversibility (3.10) is an equality:

$$J_{t,s}(\phi_t(m), \phi_s(m)) = H(\phi_t(m)) - H(\phi_s(m)), \quad t \geq s \tag{3.12}$$

Remarks on the H-theorem for irreversible dynamical systems have been written in Ref. 8.

3.1.3. Propagation of Constrained Equilibrium

The condition (3.3) of autonomy needs to be checked for all times $t \geq s \geq 0$, starting at time zero from an initial value m. Obviously, that condition is somehow related to—yet different from Boltzmann's Stosszahlansatz. The latter indeed

corresponds more to the assumption that any initial constrained equilibrium state at time zero evolves to new constrained equilibria at times $t > 0$. Formally and in the notation of Sec. 2, we consider a region M_0 in phase space corresponding to some macroscopic state and its image $f M_0$ after some time t. We then have in mind to ask that for "relevant" phase space volumes A

$$\frac{|U\ M_0 \cap A|}{|U\ M_0|} = \frac{|M_t \cap A|}{|M_t|} \tag{3.13}$$

which means that the evolution takes the equilibrium constrained with $x \in M_0$ to a new equilibrium at time t constrained at $x \in M_t$, *as far as the event A is concerned*. Indeed, we expect that one cannot distinguish M_t from $U\ M_0$ by looking at macroscopic variables. Hence the events A should correspond to values of these macroscopic variables (A_1 as defined below is an example). Since we also expect that one cannot distinguish M_t from $U\ M_0$ by studying the future evolution, A can also correspond to values of the macrovariables in the future (A_2 as defined below is an example). However, the states M_t and $U\ M_0$ can (in principle) be distinguished by looking at their past macrotrajectory. Indeed, one does not expect (3.13) to hold for $A = U\ M_0$ since the left-hand side is 1 and the right-hand side (which is dominated by $|M_0|/|M_t|$) is typically exponentially small in N.

To be more precise and turning back to the present mathematical context, we consider the following condition:

$$\lim_{\epsilon\downarrow 0}\lim_{N\uparrow\infty}\frac{1}{N}\log\frac{\rho^N\left\{x \in A_i^N \middle| m^N(x) \overset{\epsilon}{=} \phi_t(m)\right\}}{\rho^N\left\{U_t^N x \in A_i^N \middle| m^N(x) \overset{\epsilon}{=} m\right\}} = 0 \tag{3.14}$$

for all $m \in \mathcal{F}$, $t \geq s \geq 0$, $i = 1, 2$, $A_1^N \equiv \{m^N(x) \overset{\delta}{=} \phi_t(m)\}$ and

$$A_2^N \equiv \left\{m^N\left(U_t^N\left(U_s^N\right)^{-1}x\right) \overset{\delta}{=} \phi_t(m)\right\}.$$

Arguably, (3.14) is a (weak) version of propagation of constrained equilibrium. We check that it actually implies condition (3.3), and hence the H-theorem.

First, choosing $A_1^N = \{m^N(x) \overset{\delta}{=} \phi_t(m)\}$, (3.14) yields

$$\lim_{\epsilon\downarrow 0}\lim_{N\uparrow\infty}\frac{1}{N}\log\rho^N\left\{m^N\left(U_t^N x\right) \overset{\delta}{=} \phi_t(m) | m^N(x) \overset{\epsilon}{=} m\right\} = 0$$

Second, using the invariance of ρ^N,

$$\begin{aligned}&\rho^N\left\{m^N\left(U_t^N x\right) \overset{\delta}{=} \phi_t(m) | m^N\left(U_s^N x\right) \overset{\epsilon}{=} \phi_s(m)\right\}\\ &= \rho^N\left\{m^N\left(U_t^N x\right) \overset{\delta}{=} \phi_t(m) | m^N(x) \overset{\epsilon}{=} m\right\}\end{aligned}$$

$$\times \frac{\rho^N\left\{m^N\left(U_t^N\left(U_s^N\right)^{-1}x\right) \overset{\delta}{=} \phi_t(m)|m^N(x) \overset{\epsilon}{=} \phi_s(m)\right\}}{\rho^N\left\{m^N\left(U_t^N\left(U_s^N\right)^{-1}U_s^N x\right) \overset{\delta}{=} \phi_t(m)|m^N x \overset{\epsilon}{=} (m)\right\}}$$

and by applying condition (3.14) once more but now with

$A_2^N \equiv \{m^N(U_t^N(U_s^N)^{-1}x) \overset{\delta}{=} \phi_t(m)\}$ and taking the limits, we get (3.3). (Note that we have actually also used here that U_t^N is invertible or at least that $U_t^N \circ (U_s)^{-1}$, $t \geq s$ is well defined.)

3.2. Finite-Size Formulation

As announced in the questions under Sec. 2.2, we are certainly most interested in the case of finite but very large N and how the H-function can be defined along the microscopic trajectory. Consider

$$H^{N,\epsilon}(m) = \frac{1}{N}\log \rho^N\{m^N(x) \overset{\epsilon}{=} m\} \tag{3.15}$$

for (macrostate) $m \in \mathcal{F}$. For a microstate $x \in \Omega^N$, define

$$\overline{H}^{N,\epsilon}(x) = \sup_{m \overset{\epsilon}{=} m^N(x)} H^{N,\epsilon}(m)$$

$$\underline{H}^{N,\epsilon}(x) = \inf_{m \overset{\epsilon}{=} m^N(x)} H^{N,\epsilon}(m)$$

Instead of the hypothesis (3.3) of macroscopic autonomy, we assume here that there is a macroscopic dynamics ϕ_t, $\phi_0 = \mathrm{Id}$, for which

$$\lim_{\epsilon\downarrow 0}\lim_{N\uparrow\infty} \rho^N\left\{m^N\left(U_t^N x\right) \overset{\delta}{=} \phi_t(m)|m^N(x) \overset{\epsilon}{=} m\right\} = 1 \tag{3.16}$$

and that

$$\lim_{\epsilon\downarrow 0}\lim_{N\uparrow\infty} \frac{1}{N}\log \rho^N\left\{m^N\left(U_t^N x\right) \overset{\epsilon}{=} \phi_t(m)|m^N(U_s x) \overset{\epsilon}{=} \phi_s(m)\right\} = 0 \tag{3.17}$$

for all $m \in \mathcal{F}$, $\delta > 0$ and $0 \leq s \leq t$. Condition (3.16) corresponds to the situation in (3.3) but where there is a unique macroscopic trajectory, which one observes typically. Now we have

Proposition 3.2. *Assume (3.16)–(3.17). Fix a finite sequence of times* $0 < t_1 < \ldots < t_K$ *. For all* $m \in \mathcal{F}$*, there exists* $\delta_0 > 0$ *such that for all* $\delta \leq \delta_0$*,*

$$\lim_{\epsilon\downarrow 0}\lim_{N\uparrow\infty} \rho^N\left[\overline{H}^{N,\delta}\left(U_{t-j}^N, x\right) \geq \underline{H}^{N,\delta}\left(U_{t_{j-1}}^N x\right) - \frac{1}{N}, j = 1, \ldots, K|m^N(x) \overset{\epsilon}{=} m\right] = 1 \tag{3.18}$$

Proof: Put

$$g^{n,\delta,\epsilon}(s,t,m) \equiv 1 - \rho^N \left\{ m^N(U_t^N x) \stackrel{\delta}{=} \phi_t(m) | m^N(U_s x) \stackrel{\epsilon}{=} \phi_s(m) \right\} \tag{3.19}$$

then

$$\rho^N \left[m^N(U_{t_j} x) \stackrel{\delta}{=} \phi_{t_j}(m),\, j = 1, \ldots, K | m^N(x) \stackrel{\epsilon}{=} m \right] \geq 1 - \sum_{j=1}^{K} g^{N,\delta,\epsilon}(0, t_j, m) \tag{3.20}$$

Whenever $m^N(U_t x) \stackrel{\delta}{=} \phi_t(m)$, then

$$\underline{H}^{N,\delta}\left(U_t^N x\right) \leq H^{N,\delta}(\phi_t(m)) \leq \overline{H}^{N,\delta}\left(U_t^N x\right)$$

As a consequence, (3.20) gives

$$\rho^N \left[\underline{H}^{N,\delta}(U_{t_j} x) \ \leq H^{N,\delta}(\phi_{t_j}(m)) \leq \overline{H}^{N,\delta}(U_{t_j} x),\, j = 1, \ldots, K | m^N(x) \stackrel{\epsilon}{=} m \right]$$

$$\geq 1 - \sum_{j=1}^{k} g^{N,\delta,\epsilon}(0, t_j, m) \tag{3.21}$$

The last term can be controlled via (3.16). On the other hand, by the same bounds as in (3.5), we have

$$H^{N,\delta}(\phi_{t_j}(m)) \geq H^{N,\delta}(\phi_{t_{j-1}}(m)) + \frac{1}{N} \log \left[1 - g^{N,\delta,\delta}(t_{j-1}, t_j, m) \right]$$

The proof is now finished by using (3.17) and choosing δ_0 such that for $\delta \leq \delta_0$ and for large enough N (depending on δ).

$$\min_{j=1}^{k} (\log[1 - g^{N,\delta,\delta}(t_{j-1}, t_j, m)]) \geq -1$$

□

4. ADDITIONAL REMARKS

The above remains essentially unchanged for stochastic microscopic dynamics. Instead of the dynamical system (Ω, U_t, ρ) one considers any stationary process $(X_t^N)_{t \in \mathbb{R}_+}$ with the law $\mathbf{P}_N$; denote by ρ^N the stationary measure. The entropy is defined as in (3.2) but with respect to ρ^N. The (weak) autonomy in the sense of (3.3) is then

$$\lim_{\epsilon \downarrow 0} \lim_{N \uparrow +\infty} \frac{1}{N} \log \mathbf{P}_N \left[m^N\left(X_t^N\right) \stackrel{\delta}{=} \phi_t(m) | m^N\left(X_s^N\right) \stackrel{\epsilon}{=} \phi_s(m) \right] = 0$$

On the other hand some essential changes are necessary when dealing with quantum dynamics. The main reason is that, before the limit $N \uparrow +\infty$, macroscopic

variables do not commute so that a counting or large deviation type definition of entropy is highly problematic. We keep the solution for a future publication.

While some hesitation or even just confusion of terminology and concepts have remained, the physical arguments surrounding an H-theorem have been around for more than 100 years. The main idea, that deterministic autonomous equations give an H-theorem when combined with the Liouville theorem, is correct but the addition of some mathematical specification helps to clarify some points. In this paper, we have repeated the following points:

1. There is a difference between the Second Law of Thermodynamics when considering transformations between equilibrium states, and microscopic versions, also in nonequilibrium contexts, in which the Boltzmann entropy is evaluated and plays the role of an H-function.
2. The autonomy of the macroscopic equations should be understood as a semigroup property (first order differences in time) and it is a weaker condition than the one of propagation of equilibrium. Mostly, that autonomy only appears sharply in the limit of infinite scale separation between the microscopic world and the macroscopic behavior. A specific limiting argument is therefore required to combine it with Liouville's theorem about conservation of phase space volume for finite systems.

As a final comment, there remains the question how useful such an analysis can be today. Mathematically, an H-theorem is useful in the sense of giving a Lyapunov function for a dynamical system, to which we alluded in the introduction. Physically, an H-theorem gives an extension and microscopic derivation of the Second Law of thermodynamics. One point which was however not mentioned here before, was much emphasized in years that followed Boltzmann's pioneering work, in particular by Albert Einstein. The point is that one can usefully turn the logic around. The statistical definition of entropy starts from a specific choice of microstates. If for that choice, the corresponding macroscopic evolution is not satisfying an H-theorem, then our picture of the microstructure of the system is very much expected to be inadequate. In other words, we can obtain information about the microscopic structure and dynamics from the autonomous macroscopic behavior. Then, instead of concentrating on the derivation of the macroscopic evolutions with associated H-theorem, we use the phenomenology to discover crucial features about the microscopic world. That was already the strategy of Einstein in 1905 when he formulated the photon hypothesis.

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