On the ergodic hypothesis and on chaotic motions

1866 Boltzmann proposes a proof of the II law

$$\oint \frac{\mathbf{dQ}}{\mathbf{T}} \le \mathbf{0}$$

considering first a cyclic process in which

“actions and reactions are equal to each other, so that in the interior of the body either thermal equilibrium or a stationary heat flow will always be found”

We would say “evolves on a reversible cycle”

Assumption ? [1, Sec. IV,p.24]

"An arbitrarily selected atom runs, whatever the state of the system, in a suitable time interval (no matter if very long), of which the instants t_1 and t_2 are the initial and final times, at the end of which the speeds and the directions come back to the original value in the same location, describing a closed curve and repeating, from this instant on, their motion."

The proof is developed imagining that the entire system moves on a periodic motion. Same assumption in Clausius,[2]: different path from Maxwell, [3].

Should be read as "things go as if ...".

I.e. the second law follows from mechanics as a unversal property of Hamiltonian periodic motions, it is like a "symmetry".

Heat theorem arises as a property of the variation $\delta(\overline{K} - \overline{V})$ btwn motion x and varied motion x'

$$\mathbf{x}(\mathbf{t}) = \mathbf{x}(\mathbf{i}\varphi) \stackrel{\mathbf{def}}{=} \boldsymbol{\xi}(\varphi), \qquad \mathbf{t} \in [\mathbf{0}, \mathbf{i}],$$

$$\mathbf{x}'(\mathbf{t}) = \mathbf{x}'(\mathbf{i}'\varphi) \stackrel{\mathbf{def}}{=} \boldsymbol{\xi}'(\varphi), \quad \mathbf{t} \in [\mathbf{0}, \mathbf{i}'], \qquad \delta\mathbf{i} = \mathbf{i}' - \mathbf{i}$$

Energy (average over period) varies by δU and δQ is the heat received

$$\delta\mathbf{U} = \delta(\overline{\mathbf{K}} + \overline{\mathbf{V}}), \qquad \delta\mathbf{Q} = \delta\mathbf{U} - \overline{\delta\mathbf{V}}_{\mathbf{ext}}$$

Compute, $\delta(\overline{K} - \overline{V})$ as usual in least action p. (exercise)

$$\delta(\overline{\mathbf{K}} - \overline{\mathbf{V}}) + \overline{\delta\mathbf{V}}_{\mathbf{ext}} + \mathbf{2}\overline{\mathbf{K}}\delta\log\mathbf{i} = \mathbf{0}$$

$$+\,\mathbf{2}\delta\overline{\mathbf{K}} - \delta(\overline{\mathbf{K}} + \overline{\mathbf{V}}) + \overline{\delta\mathbf{V}}_{\mathbf{ext}} + \mathbf{2}\overline{\mathbf{K}}\delta\log\mathbf{i} \;=\; \mathbf{0}$$

$$-\delta\mathbf{Q} + \mathbf{2}\,\delta\overline{\mathbf{K}} + \mathbf{2}\,\overline{\mathbf{K}}\,\delta\log\mathbf{i} \equiv -\delta\mathbf{Q} + \mathbf{2}\,\overline{\mathbf{K}}\,\delta\log(\overline{\mathbf{K}}\mathbf{i}) = \mathbf{0}$$

$$\Rightarrow \quad \frac{\delta\mathbf{Q}}{\overline{\mathbf{K}}} = \mathbf{2}\,\delta\log(\overline{\mathbf{K}}\mathbf{i}) \stackrel{\mathbf{def}}{=} \delta\mathbf{S}$$

”It is easily seen that our conclusion on the meaning of the quantities that intervene here is totally independent from the theory of heat, and therefore the second fundamental law is related to a theorem of pure mechanics to which it corresponds just as the “vis viva” principle corresponds to the first principle; and, as it immediately follows from our considerations, it is related to the least action principle, in a somewhat generalized form.” [1, #2,sec.IV]

In 1868 B. discovers the microcanonical ensemble.

In Sec. III,IV **changes completely the point of view: from kinetic theory of Maxwell (in infinite homogeneous systems) attacks the problem of finite systems.**

First considers particles interacting via forces of very short range (⇒ collisions duration neglegible) then considers the general case:

Two key ideas (1868), [4]**:**

(1) all microscopic states will be visited in the course of time (now periodicity appears as hypothesis that the entire energy surface is visited).

(2) The microscopic states are represented through cells in phase space ("cubic")

Periodicity ⇒ the weight of each micr. configuration ≡ number of ways to realize it, "permutability". Well known to imply microcanonical ensemble)

$$\mathrm{const}\ \delta\Big(\frac{1}{2}\sum_i \tilde{k}_i^2 + V(\tilde{q}_1, \cdots, \tilde{q}_N) - NE\Big)\ d^3\tilde{k}_1 \cdots d^3\tilde{q}_N$$

In the literature this work is often ignored and some of the ideas are referred to the later 1877 paper, [5].

In 1871 Trilogy B.[6, 7, 8], is possibly unhappy about the discretization

Studies the distribution of the atoms of each single molecule in a gas

“it is not unreasonable” to think that, in a gas in equilibrium, each moves visiting all possible microscopic states

Following Maxwell, derives by compatibility with the conservation laws, the distribution must be a function of the constants of motion (just one) and of the form $\mathbf{e^{-h(K+V)}}$ (smoothness assumed)

But a terrible doubt arises as multiple collisions have been negelcted:
Against me is the fact that, until now, the proof that these distributions are the only ones that do not change in presence of collisions is not complete, [6, p.255,l.21]**.**

In II of trilogy deals with an entire system of N atoms without neglecting multiple collisions: it is to be considered as a giant molecule.

But to reduce to preceding case needs hypothesis:[7, III,p.284]

The great chaoticity of the thermal motion and the variability of the force that the body feels from the outside makes it probable that the atoms get in the motion, that we call heat, all possible positions and velocities compatible with the equation of the kinetic energy, and even that the atoms of a warm body can take all positions and velocities compatible with the last equation considered.

If all permitted configurations are visited (periodicity is implied) and the distribution is continuous (hence > 0) then it must be the uniform distribution, *i.e.* microcanonical.

This is the ergodic hypothesis: without recourse to external stochastic forces, and Maxwell tributes a great recognition to the 1868 paper where it an be traced, as follows [9, p.734]:

"The only assumption which is necessary for the direct proof [of the microcanonical distribution by Boltzmann] **is that the system, if left to itself in its actual state of motion, will, sooner or later, pass through every phase which is consistent with the equation of energy. Now it is manifest that there are cases in which this does not take place**
... But if we suppose that the material particles, or some of them, occasionally encounter a fixed obstacle such as the sides of a vessel containing the particles, then, except for special forms of the surface of this obstacle, each encounter will introduce a disturbance into the motion of the system, so that it will pass from one undisturbed path into another...."

In the 3d 1871 paper appears notion of mechanical model of Thermodynamics and the theory of ensembles is developed to leave aside the 2 hypotheses on the microscopic dynamics.

It is shown possible to define distributions attributing to some mechanical observables average values, to be called U, V, p, T so that, varying the distribution (*i.e.* the macroscopic state), the averages U e V vary while the differential

$$\frac{\mathbf{dU + pdV}}{\mathbf{T}}$$

is exact.

There are several models ("ensembles") of Thermodynamics. The ergodic hypothesis guarantees that one is physically relevant for Thermodynamics: others are equivalent to it.

However if we only look for models it is no longer necessary! Ensebles theory is born. But Erg. hyp. is still needed.

This is the starting point of the pragmatic Gibbs.

The E. hypothesis has been criticized as mathematically inconsistent: easy to see.

Question: MS founded while ignoring this ? possible ??

The 1868 discrete derivation of the m. ens. provides a clear answer.

B. (and M.) had a discrete conception of phase space and time; then:

(1) The hypothesis, *i.e.* point visits the entire energy surface, in B.&M. not absurd if space is imagined discrete

(2) Recurrence times are superastronomical but the small number and the nature of relevant observables greatly reduces to a human scale the times of approach to equuilibrium, as discussed by B. and Thomson

(3) Ensembles are independent from the ergodic hypothesis

(4) A discrete representation presupposes a phase space discretized on a regular lattice; hence the special stats assigned to the Liouville's measure; it appears as an "experimental datum" due, perhaps, to our perception of (local) space-time as a translationally invariant continuum.

(5) The ergodic h. selects uniquely the only distributions describing macroscopic Thermodynamics.

Thus B.'s point: Hamiltonian systems provide examples no matter whether they contain $N = 1$ or $N = 10^{19}$, accepting the ergodic hypothesis (hence periodicity).

Discrete phase space? Really ?? Quotations without comments

For instance, [10, p.169]**:**

... if we wish to get a picture of the continuum in words, we first have to imagine a large, but finite number of particles with certain properties and investigate the behavior of the ensemble of such particles. Certain properties of the ensemble may approach a definite limit as we allow the number of particles ever more to increase and their size ever more to decrease. Of these properties one can then assert that they apply to a continuum, and in my opinion this is the only non-contradictory definition of a continuum with certain properties

E [10, p.55]**:**
Through the symbols and manipulations of integral calculus, which have become common practice, one can temporarily forget the need to start from a finite number of elements, that is at the basis of the creation of the concept, but one cannot avoid it.

E [10, p.56]:

The concepts of differential and integral calculus separated from any atomistic idea are truly metaphysical, if by this we mean, following an appropriate definition of Mach, that we have forgotten how we acquired them.

O [10, p.55-56]:

Often ... it is necessary to put aside the basic concept, from which they have overgrown, and perhaps to forget it entirely, at least temporarily. But I think that it would be a mistake to think that one could become free of it entirely.

O [10, p.227]:

"...we cannot exclude the possibility that for a certain very large number of points the picture will best represent phenomena and that for greater numbers it will become again less accurate, for atoms do exist in large but finite number.

Natural question: Ergodic h. is also relevant for stationary states out of equilibrium ? So B., [11, p.218]:

Let us think of an arbitrarily given system of bodies, which undergo an arbitrary change of state, without the requirement that the initial or final state be equilibrium states; then always the measure of the permutability of all bodies involved in the transform. continually increases and can at most remain constant, until all bodies during the transform. are found with infinite approximation in thermal equilibrium.

Begin by stressing that Liouville's th. although guaranteeing invariance of the micr. can. distribution does NOT imply that it is the equil. distr.

Except exceptions, chaotic dyn. sys. admit uncountably many invariant distrib.. Anyway out of equil. Liouville's th. cannot be applied:

⇒ discrete phase space view needs to be reconsidered.

Possible for particularly simple systems: the hyperbolic systems (or for Anosov systems).

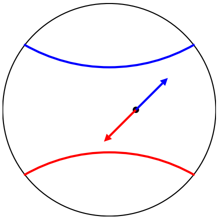
The idea is: assume that a system of particles is such; just as in equilibrium it had been supposed that atoms of a macroscopic body move periodically.

Aim: exhibit properties general and common to hyperbolic sys., considering them as paradigm of chaotic systems. This is the chaotic hypothesis.

In a continuous representation of phase space dissipation ⇒ time average of volume contraction is $\sigma_+ > 0$ positive.

⇒ motions tend asymptotically to an attracting set $\mathcal{A}$ and on it to the attractor $\mathcal{B}$ (with 0 vol).

In general nonconserv. motions, *nonrecurrent points will be "most" points*: $\mathcal{A} =$ may be entire phase space, but $vol(\mathcal{B}) = 0$.

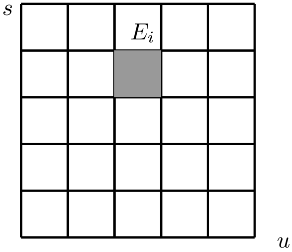


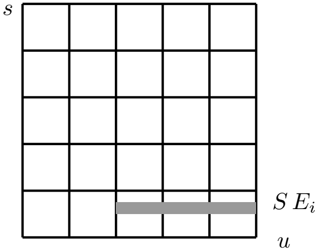
For simplicity observations will be made at timing events, *i.e.* when a prefixed event occurs: in this way motion is described by the map S trasforming x to the next S x.

Key property of hyperb. sys.: possibility of a partition in cells with remarkable properties, named Markovian.

At each point of a hyperb. sys. depart two surfaces ("stable and unstable") which S expands or contracts

They can be used to form cells $E(q)$: *i.e.* domains (symbolically drawn as squares) with boundaries consisting of surface elements which under the evolution dilate or contract. They can be imagined to be foliated by surface elements of either type.





their boundaries enjoy a covariance property

To each point x in phase space corresponds a sequence

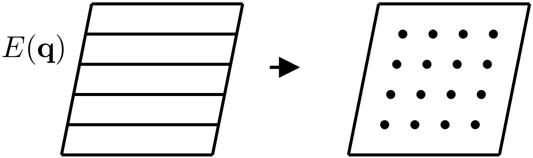
$$\boldsymbol{\sigma} = \{\sigma_j\}_{j=-\infty}^{\infty} = (\ldots, \sigma_{-1}, \sigma_0 \sigma_1, \ldots)$$

if at time j the point x evolved falling in $S^j x \in E_{\sigma_j}$.

The discrete reprresentation is without constraints, other than the obvious condition that symbol $\sigma' = \sigma_{j+1}$ can follow $\sigma = \sigma_j$ only if SE_σ intersects $E_{\sigma'}$: an event denoted $T_{\sigma,\sigma'} = 1$ or $T_{\sigma,\sigma'} = 0$ otherwise.

Absence of constraints is due to the covariance. Leads to many properties of invariant distributions (∞-many).

The attractor $\mathcal{B}$ is associated with the unstable surfaces and in a regular lattice discretization of the attractine set it becomes a finite number of points.



All initial data end up, after a transient as points of the attractor $\mathcal{B}$: which will be a subset (often very small) of oints of the attracting set $\mathcal{A}$.

In analogy to ergodic hypothesis it can be imagined that attractor points move on a single periodic path.

If $\sigma(q)$ is the unstable surfaces size in $E(q)$, the number of points of the attractor will be $\mathcal{N}(q) = \rho(q)\sigma(q)$ and the density $\rho(q)$ will satisfy (compatibility in=out)

$$\rho(q) = \sum_{q'} e^{-\lambda_i(q')}\rho(q')T_{q,q'}, \qquad T_{q.q'} = 0, 1$$

This is a heuristic interpretation of the (non trivial) general properties of mixing in Anosov systems.

Hence motion on the attractor $\mathcal{B}$ is periodic and the stationary distribution simply assigns the same weight ($i.e.$ $1/\mathcal{N}$) to the attractor points. Manifestly unique.

This distribution is the SRB distr. introduced by Ruelle, [12], as the natural distribution for the statistics of chaotic motions: it is the SRB distribution.

If the discretization is on a regular lattice, in the Hamiltonian case and if the attractor is identified with the attracting set ($i.e.$ the energy surface) the microcanonical distr. is obtained. Any distinction between Hamiltonian and dissipative systems disappears and in all cases statistics is determined by the uniform distribution (as in 1868) on the attractor.

It remains to explain: why a unique distribution is found while it is well known that hyperbolic sytems admit uncountably many invariant ones?

Reflects discretization is on a regular lattice. Had it been performed on a non regular lattice,with fractal properties, via same arguments and same ergodicity assumption other distr., also unique, $\neq SRB$, arise.

Validity of the theory, in and out of equilibrium, is an "experimental confirmation" of our perception of the local continuum as a translation invariant space, [13, 14].

And Entropy ? next time

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and, in parentheses, to the collected works

http://ipparco.roma1.infn.it/∼giovanni

$$
\begin{aligned}
x(t) =& \xi(\frac{t}{i}), \qquad \dot{x}(t) = \frac{1}{i}\partial_\varphi \xi(\frac{t}{i}) \\
x'(t) =& \xi'(\frac{t}{i'}), \qquad \dot{x}'(t) = \frac{1}{i'}\partial_\varphi \xi(\frac{t}{i'}) \\
\xi'(\varphi) =& \xi(\varphi) + \Delta(\varphi) \\
V'(\varphi) =& V(\varphi + \Delta(\varphi)) + \delta V_{ext}(\varphi + \Delta(\varphi))
\end{aligned}
$$

$$
\begin{aligned}
\delta(\overline{K} - \overline{V}) = & \int_0^1 \frac{1}{2}((\frac{1}{i'}\partial_\varphi x'(\varphi))^2 - (\frac{1}{i}\partial_\varphi x(\varphi))^2 - (V'(\xi'(\varphi)) - V(\xi(\varphi))))\, d\varphi \\
& - 2\frac{\delta i}{i}\overline{K} + \int_0^1 d\varphi \Big[\frac{1}{2i^2}((\partial_\varphi \xi')^2 - (\partial_\varphi \xi)^2) - (V(\xi + \Delta) + \delta V(\xi) - V(\xi))\Big] \\
& = -2\frac{\delta i}{i}\overline{K} - \bar{\delta} V_{ext}
\end{aligned}
$$