Ergodicity: an early paper by Boltzmann and its relevance

The "second law": $\oint \frac{dQ}{T} = 0$ & $\oint \frac{dQ}{T} \leq 0$
In 1866 Boltzmann develops the idea that second law reflects a very general property of Hamiltonian mechanics, $\Rightarrow$ "theorem"

The basic assumption [1, Sec. IV,p.24], is that

" *We shall now suppose that an arbitrarily selected atom moves, whatever is 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* "

Fundamentally motions are periodic: $\Rightarrow$ averages computed simply by integrating over the period *i.e.* over the phase.

Let δx be the variation that the motion $t \to x(t)$ undergoes in

"*a process in which actions and reactions during the entire process are equal to each other so that in the interior of the body either termal equilibrium or a stationary heat flow will always be found*",[1].

The heat theorem then becomes a property of the variation $\delta(\overline{K} - \overline{V})$, $V = V_{int} + V_{ext}$. B. assumes $V_{ext} = 0$ and $\delta Q = \delta U - \overline{\delta V}_{ext}$ is interpreted as heat received as $x \to x'$. Setting $V_{ext} = 0$ it follows that, *if the eq. of motion hold*

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

Clausius complains that $V_{ext} = 0$, B. says yes but the argument would be the same, Clausius says no ... Both agree that the second law is an expression of the "least action principle" and is a theorem.

”*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]

“Generalization of the action principle” ???:

However the priority issue (1871) was secondary, given the new developments by B.: In 1868 he had derived the canonical distribution for the statistics of the atoms of a molecule in a gas in termal equilibrium.

First he considers a very rarefied gas with molecules experiencing instantaneous collisions (constant kinetic energy): deriving their canonical distribution. Then he derived the microcanonical distr. for the entire gas (as a giant molecule).

Here for the first time the phase space is imagined divided into cells and the distribution is derived by counting the number of ways to distribute particles in the cells ($6N$-dimensional) of given total energy: dynamics enters only because it is supposed that the system takes periodically all possible configurations.

But in Sec.III of the paper the rarefied gas assumption is removed and analysis becomes really general with an internal potential energy $\chi(q)$ "arbitrary".

Phase space of total energy $n\kappa$ is divided into cells $d^{3N}q d^{3N}p$ and for each $q \in R^{3N}$ the cells $d^{3N}p$ available (*i.e.* with $K = n\kappa - \chi(q)$): distributing particles in them gets (translated to modern notations):

$$\frac{\delta(n\kappa - \frac{1}{2}p^2 - \chi(q))\; d^{3N}q d^{3N}p}{norm}$$

$\to$ microcanonical distribution, *e.g.* $(n\kappa - \chi(q))^{\frac{3n-2}{2}} \frac{d^{3n}q}{norm}$ if integrated over p's.

The argument is combinatorial and dynamics enters only because all ways of filling the cells with particles are visited once per periodic cycle of the system: Ergodic hypothesis.

So Maxwell in one of his last papers, [5]:
" *The only assumption which is necessary for the direct proof 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...."

It might take a long time to do so but eventually it will be repeated.

So the most urgent problem was to convince skeptics (not yet in great number at the time, 1868) that (generically) an unperturbed motion would wander in phase space visiting all points of given energy: and "all" has to be intended keeping in mind that phase space is discrete.

Boltzmann needed at least one simple example with more structure than the quasi periodic Lissajous curves: *i.e.* a Hamiltonian system with orbits dense on the energy surface.

Under the unassuming title "Solution of a mechanical problem" [2] ("Lösung eines mechanisches Problems", 1868) he considers a point moving under a gravitational attraction potential $-\frac{\alpha}{2r}$ and a centrifugal potential $\frac{\beta}{2R^2}$. The aim being to manufacture one example, given that it is "not really easy to find" one (!).

This is a Hamiltonian with 2 degrees of freedom that admits energy and angular momentum conservation and can be solved by elementary quadrature: all its motions are quasi-periodic aside from special cases (resonances).

The Hamiltonian is

$$H = \frac{1}{2}p^2 - \frac{\alpha}{2R} + \frac{\beta}{2R^2}$$

And if the polar coord. at time t are $t \to (r(r), \varphi(t))$ in a motion with energy $\frac{1}{2}A < 0$ and angular momentum a then

$$\varphi(t) = \varphi(0) + F(r(t), a, A) - F(0, a, A) \equiv \varepsilon + F(r(t), a, A)$$

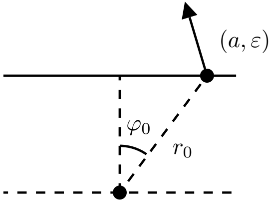
$$F(r, a, A) = \frac{a}{\sqrt{a^2 + \beta}} \arccos\Big(\frac{2(a^2 + \beta)/r - \alpha}{\sqrt{\alpha^2 + 4A(a^2 + \beta)}} \Big)$$

Likewise the case of a centrifugal potential $\frac{\beta}{2R^2}$ and of a harmonic potential $\frac{1}{2}\kappa R^2$ can be considered (Botlzmann did consider it in other papers).

$$H = \frac{1}{2}p^2 + \frac{\kappa}{2}R^2 + \frac{\beta}{2R^2}$$

Elementarily integrable and all motions are quasi periodic.

Then Boltzmann imagines to put a barrier at height y:



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and the particle, imagined as living above the obstacle, is reflected elastically at each collision.

Angular momentum is no longer conserved and collisions take place in a 2 dimensional space. Conveniently studied in the coordinates (a, φ) of successive collisions (Poincaré' map). Or also (x, a) with $x = y \tan \varphi$: so the evolution becomes a map $(x, a) \to (x', a')$.

The idea, and B.'s conclusion, seems that, angular momentum being not conserved, the formerly quasi periodic motion will invade densely the energy surface (later this will be formalized as the "quasi ergodic hypothesis", by Ehrenfests).

In detail B. proves that there is an invariant density: he gets this via what we call the Liouville's theorem (which in his works he proves every time he needs it via explicit often very long calculations).

Then he assumes that the number of events (*i.e.* visits) in $dadx$ has the form

$$F(a, x)dadx$$

(we say the visit probability is absolutely continuous).

Concludes that F is the frequency of visit apparently taking for granted that F is continuous on the densely covered energy surface. As done again and again later (and earlier).

Summarizing B. already in the earlier work and in all successive ones was assuming that 1) motions cover densily the energy surface and, 2) they visit regions with a density function which is continuous.

Is this true? I doubt.

The system is very simple and a simulation is possible: the results are quite surprising.

Left is gravitation + centrigugal forces case and the right is harmonic+centrifugal, in the x, a plane:

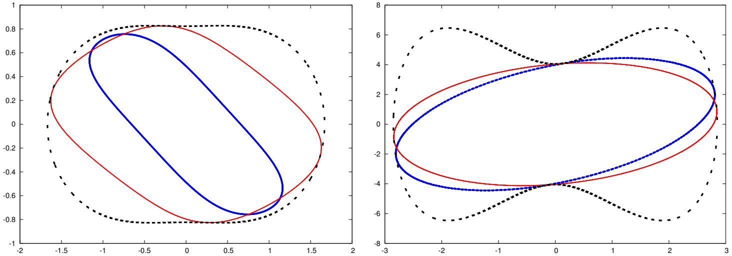

fig.4

Energy surface at collisions is enclosed by the dotted curve.
Curves are two trajectories with equal energy

Definitely not ....

But I chose parameters $y = 1$ (quota of obstacle), and $\beta = .1$ (centrifugal coupling) quite small. Ian Jauslin instead tested β large (~ 10 times my value) and found that the motion was invading an open region of phase space.

In this case B. seemed right.

Why did Boltzmann introduce the centrifugal force? maybe to make sure that at least in absence of the obstacle the motions were already quasi-periodic?

I have studied the problem with $\beta = 0$ (no centrifugal force) and it seems that the motions in the Poincaré map plane (a, e or a, e) are always running on closed orbits (except at resonances where they consist of finitely many points).

Can one make a theory of the above phenomenology?

Yes (or maybe)

Conjecture

In absence of centrifugal force the system is integrable for all y

Notice that this is trivially true if $y = 0$.

If true this would be a beautiful property of **conic sections**: the orbits between collisions are elements of a family of conics (ellipses) confocal and coaxial (*i.e.* of equal major axis).

The conjecture would imply that the collision points (x, a) are located on closed curves in the x, α-plane. If true maybe Apollonius knew that? Families of confocal conics have a large number of geometric properties if also coaxial should have more.

If the conjecture is correct then the figures above would be "immediate" consequences of the KAM theorem (in Moser's version) for β is small: and the chaos observed at large β should be part of the Aubry-Mather theory.

If not there is still hope that KAM theorem could say something at least when the parameters y and β are small.

In the oscillator case analysis is similar: the case of no centrifugal force gives a family of concentrical ellipses (rather than confocal) which kight be easier.

Conclusion: Boltzmann's hope that his would be a simple example of a chaotic system seems not always right. But even where it is not so his intuition of the importance of the centrifugal force may be basically correct and hide a new elementary integrable system with a chaotic transition.

[3, 4]

[1] L. Boltzmann.

Über die mechanische Bedeutung des zweiten Hauptsatzes der Wärmetheorie.

Wiener Berichte, 53, (W.A.,#2):195–220, (9–33), 1866.

[2] L. Boltzmann.

Lösung eines mechanischen problems.

Wiener Berichte, 58, (W.A.,#6):1035–1044, (97–105), 1868.

[3] G. Gallavotti.

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[4] G. Gallavotti.

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Eur. Phys. J. H., 41, online-first:1–80, 2016.

[5] J. C. Maxwell.

On Boltzmann's theorem on the average distribution of energy in a system of material points.

Transactions of the Cambridge Philosophical Society, 12:547–575, 1879.