Ergodicity: an early paper by Boltzmann and its relevance

The "second law": $\oint \frac{dQ}{T} = 0$ & $\oint \frac{dQ}{T} \le 0$
In 1866 Boltzmann developed the idea that the second law reflects a general property of Hamiltonian Mechanics, ⇒ hence it becomes a "theorem"

The basic assumption, [1, Sec. IV,p.24], was:

" *We shall now suppose that an atom, arbitrarily selected, whatever is the state of the system, in a suitable time interval (it does not matter if it is very long) of which t_1 and t_2 are the initial and final instants, at the end of which the speeds and directions return to the original value, describing a closed curve and repeating, from these instants onward their motion.*"

Fundamentally motions are periodic: ⇒ averages are then simply evaluated by integration over the period, *i.e.* over the phase.

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

"*a process in which actions and reactions are, during the entire process, reciprocally equal so that in the body interior one finds always thermal equilibrium or a stationary heat flux*" [1].

The 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 if $x \to x' = x + dx$.
Taking $V_{ext} = 0$ it follows, *from the equations of motion*

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

Clausius criticizes $V_{ext} = 0$, B. admits but says that the argument would not change, Clausius says no ... Both agree that the law is an expression of the " minimal action principle" which implies it as a theorem:

"*It is easily seen that our conclusion on the significance of the quantities intervening here is totally independent from the theory of heat, and therefore the second fundamental law is related to theore of pure Mechanics to which it corresponds just as the "live force principle corresponds to the first law; and, as it follows immediately from oour considerations, it is related to the a somewhat generalized form of the least action principle.*", [1, #2,sec.IV]

""Generalization of the action principle" ???:

But the priority dispute, (1871), remained secondary, because of the new developments by B.: in 1868 derived the canonical distribution for the statisticcs of monomolecular atoms in thermal equilibrium.

Considers first a very rarefied gas in which some molecules (*e.g.*one) collide with the others and deducts their canonical distribution. Then deduces the microcanonical for the entire gas (seen as a giant molecule).

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

BUT in Sec.III also the rarefied gas hypotesis is removed and the analysis becomes really general with and internal potential energy $\chi(q)$ "arbitrary".

Phase space of total energy $n\kappa$ is divided into cells $d^{3n}qd^{3n}p$ and for each $dq \in R^{3n}$ the allowed cells $d^{3n}p$ (*i.e.* with $K = n\kappa - \chi(q)$) contain (literally although expressed in modern notationn)

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

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

The argument is combinatorial and dynamics intervenes only because all ways of locating atoms in the cells are realized only once every period cycle: ergodic hypothesis.

So Maxwell comments B. in one of his last papers, [3]:
"*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...."

A long time might be needed but eventually the cicloi will be repeated.

Therefore the most urgent problem of B. was to convince skeptics (not yet in large number, 1868) that (generically) an unperturbed motion would roam in phase space visiting all points of equal energy: and of course by "all" one has to understand it by keeping in mind a discrete phase space.

Boltzmann needed al least a simple example of motion which would visit densely the accessible: *i.e.* a Hamiltonian system with orbits covering densely the energy surface. It should be stressed that B. considered that the equilibrium distribution had a regular density, hence a distribution with regular density on a dense set and in absence of other constants of motion had to be microcanonical.

Under the modest title "Solution of a mechanical problem" [2] ("Lösung eines mechanisches Problems", 1868) considers a point in motion under a gravitationsl potential $-\frac{\alpha}{2r}$ and a centrifugal potential $\frac{\beta}{2r^2}$. The purpose is to build an example, since this is "not really easy to find" **(!)**.

This is a Hamiltonian system, 2 degrees of freedom admitting energy and angular momentum conserved, soluble via elementary quadratures: all its motions are quasi-periodic aside special cases (resonances). The Hamiltonian is

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

If the polar coordinates at time t are $t \to (r(r), \varphi(t))$ for a motion with energy $\frac{1}{2}A < 0$ and angular momentum a:

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

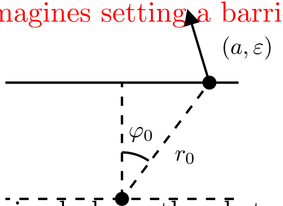
$$F(r, a, A) = \frac{a}{\sqrt{a^2 + \beta}} \arccos\Big(\frac{2(a^2 + \beta)/r - \alpha}{\sqrt{\alpha^2 + 4A(a^2 + \beta)}}\Big)$$

Likewise one can consider the case of a harmonic potential $\frac{1}{2}\kappa r^2$ and a centrifugal potential $\frac{\beta}{2r^2}$ (Botlzmann did consider it later):

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

also elemtarily integrable with all motions quasi periodic.

Then Boltzmann immagines setting a barrier at height y:



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

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

The idea and conclusion of B.'s seems to have been that, given the non conservation of the angular momentum, the formerly quasi periodic motion will invade densely the energy surface; (later this will be formalized as "quasi ergodic hypothesis", by the Ehrenfests).

In detail B. proves the existence of an invariant density: this is obtained via Liouville's theorem (which in his works is derived every time needed 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 that the probability of visit is absolutely continuous).

Concludes apparently taking for granted that F is continuous on the enery surface, densely covered by the motion, as done several times in subsequent (and preceding) works. And that there are no other such invariant distributions.

Summary: B. already in the earlier works and in all susequent ones supposed
1) motions err densely on the energy surface and
2) visit regions with a density F which is continuous
(3) Generically F is a function of the energy.

Is this true here? **doubt**.

System is very simple and a simulation is possible: with results somewhat surprising.

Left is the gravitation + centrifugal, right case is harmonic+centrifugal, in the x, a coordinates:

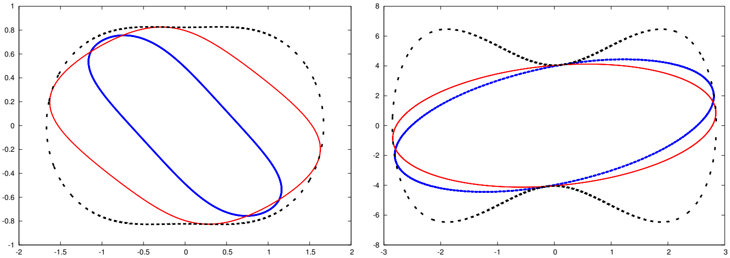


fig.4

The dashed line encloses the energy surface, at collisions, Le curves are two distinct equal energy trajectories

It seems not ....

However parameters are $y = 1$ (obstacle quota), and $\beta = .1$ (centrifugal, rather small) and $\alpha = 1$ (gravity). Ian Jauslin instead took β larger (~ 10 times) finding that notion invaded an open region of the energy surface.
In the latter case B. seems right.

Why does B. introduce the centrifugal (or harmonic) force? perhaps to make sure that in absence of the obstacle motions were already quasi periodic? or because he suspected that without centrifugal force motions still remained quasi periodic?

Studying the problem with $\beta = 0$ (no centrifugal f.) it appears that the motions in the Poincaré plain (a, e or a, e) always run on closed, hence not dense (except in resonant cases in which they consist of a finite number of points).

Is it possible to formulate a theory of the descibed phenomenology?

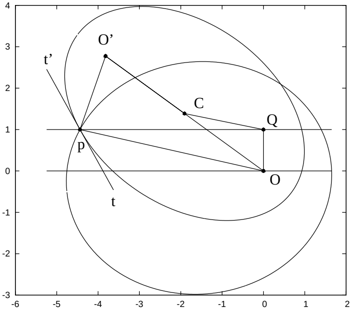
Yes (perhaps)

Conjecture (B. ?)
In absence of centrifugal f. the system is integrable and anisochronous for all $y > 0$. Trivial if $y = 0$.

If true it would reflect a nice property of conic sections: between collisions the orbits form a family of conics (ellipses) $\frac{1}{2}$-confocal and coaxial (*i.e.* a common focus and equal major axes). Conjecture would imply that the collision points (x, a) are located on closed curves in the x, α plain. Perhaps Apollonius knew? Families of confocal conics share many geometrical properties; if also coaxial have more but what about the $\frac{1}{2}$-confocal?

If conjecture is correct the shown figures would be consequences of the KAM theorem (in Moser's version) for β small: and the observed chaos at large centrifugal β would belong to theAubry-Mather theory.

A property that emerges easily in simulations (discovered by I.Jauslin) leads to the following theorem (G.-J.)':



Theorem 1: *Let $\mathcal{E}$ be an ellipse with major semiaxis a_M, aphelion inclination φ_0 and focus in O: the ellipse center C is at a distance R_0 from Q depending only from $\cos(2\lambda)$ with λ the angle formed by the tangent to $\mathcal{E}$ at the intersection with $\mathcal{L}$ and $\mathcal{L}$ itself.*

Corollary: *The angular momentum a, the aphelion angle φ_0 and*

$$\begin{aligned} R_0^2 =& \frac{1}{4} r_0^2 + \frac{1}{4}(2a_M - r_0)^2 + \frac{1}{2} r_0 (2a_M - r_0)\cos(2\lambda_0) \\ R =& a_0^2 + e_0 h\alpha \sin\varphi_0, \qquad e_0 = \sqrt{1 + \frac{4Aa_0^2}{\alpha^2}} \end{aligned} \tag{0.1}$$

with $e =$ eccentricity $e = \sqrt{1 + \frac{4Aa^2}{\alpha^2}}$, define a constant of motion R_0, which can also be written as R.

Hence, given the other constant energy, motion is represented as a curve (*i.e.* $R = const$). The question is then which is the angle conjugated to the constant R ?

There should exist an angle θ which at each collision advances by a constant rotation ω.

I. Jauslin has proposed that the angle could be simply the angle variable of the Hamiltonian R with (a_0, φ_0) as conjugated variables:

$$R = a_0^2 + e_0 y \alpha \sin\varphi_0, \qquad e_0 = \sqrt{1 + \frac{4Aa_0^2}{\alpha^2}}$$

where φ_0 is the aphelion inclination over the x-axis of the ellipse emerging from the collision x_0 and e_0 is its eccentricity, R is the above expression of the constant of motion.
Apparently this Hamiltonian bears *no relation* with our dynamics. Still it is integrable by quadrature. Let I, γ be its action-angle variables with

$$I = \int_0^{2\pi} a_{A,R}(\psi) d\psi, \qquad \gamma(\varphi_0) = \partial_R \int_0^{\varphi_0} a_{A,R}(\psi) d\psi$$

Let φ, φ' the aphelions in 2 successive collisions and let $\theta(A, R)$ be time btw collisions and $\tau(A, R)$ period in absence of coll., then

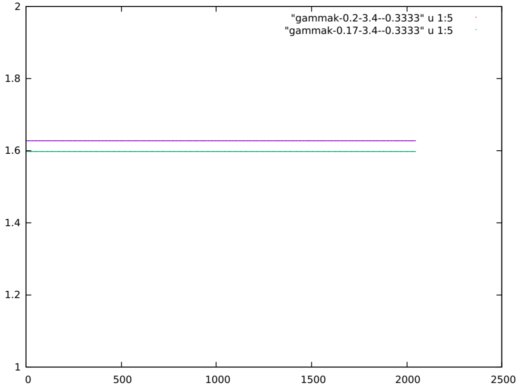
$$\gamma' = \gamma + \omega(A, R), \qquad \omega(A, R) = 2\pi \frac{\theta(A, R)}{\tau(A, R)}$$

Conjecture: $\omega(A, R)$ does not depend on the collisions if the circle, on which the centers move, contains the focus, furthermore $\partial_R \omega(A, R) \neq 0$.

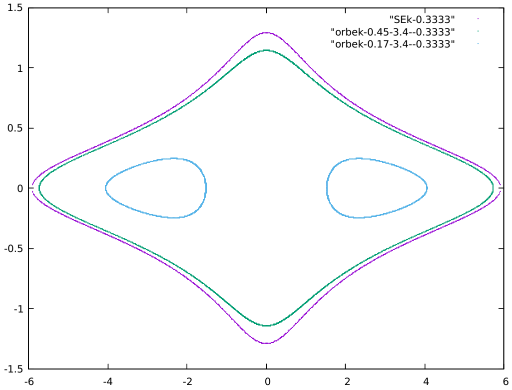
If so I, γ appear as a pair of integrating coordinates. The $\omega(A, R)$ can be expressed via elliptic integrals and its collision independence would be a further identity between elliptic integrals. Simulations apparently agree with the conjecture.

Conclusion: Boltzmann's proposal that this could be a simple example of chaotic system if $\beta \neq 0$ does not seem always correct. But even if not correct his intuition about the importance of the centrifugal force might be fundamentally right and lead to a new integrable system with a chaotic transition in presence of pertubations.

If $R < y\alpha$ the circle of the centers of the ellipses is not covered densely by the trajectory: motion is like a that of a pendulum. In this case the I.J. formula does not seem to be valid.



$\omega(A, R)$ in 2000 iterations each consisting of two successive collisions (J.Jauslin conjecture)



Orbits: in (x, u) coordinates the external curve encloses all points of given energy A; the first from the outside is connected; the second is an rbit with smaller ellipses (*i.e.* smaller A) which appears disconnected in two lines. As the maximum of the elongation decreases (*i.e.* as $R\downarrow$) the connected orbits becomes disconneted.

[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] 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.

On the other hand the center C can also be determined from the aphelion angle φ_0 and a, e as

$$C = e\, a_M(\cos\varphi_0, \sin\varphi_0)$$

so that (Cauchy's th.) $R_0^2 = e^2 a_M^2 + h^2 - 2ea_M h \sin\varphi_0$ is a constant of motion as well as

$$\frac{R_0^2 - h^2 - a_M^2}{a_M} = (e^2-1)a_M - 2eh\sin\varphi_0$$

(since a_M and h are given constants).
Hence, by Kepler's law "$G^2 = (1-e^2)L^2$", which in our notations becomes $a^2 = (1-e^2)\frac{\alpha^2}{-4A}$:

Corollary: *The angular momentum a, the aphelion angle φ_0 and*

$$R = a^2 + h\alpha e \sin\varphi_0 \equiv -\frac{\alpha}{2a_M}(R_0^2 - h^2 - a_M^2)$$

where e is the eccentricity $e = \sqrt{1+\frac{4Aa^2}{\alpha^2}}$, define constants of motion R, R_0.

$$a_{\pm}^2 = 2Ay^2 + R \pm \sqrt{4A^2y^4 + 4Ay^2R + \alpha^2y^2}$$

$$\tau(A,R) = 2\int_{a_-}^{a_+} \frac{da}{\sqrt{\alpha^2y^2 - R^2 + (4Ay^2 + 2R)a^2 - a^4}}$$

$$\gamma' = \gamma + \omega(A,R), \qquad \omega(A,R) = 2\pi\frac{\theta(A,R)}{\tau(A,R)}$$

time θ between collisio

$$\theta = \int_{a_1}^{a_0} \frac{da}{\sqrt{(a_+^2 - a^2)(a^2 - a_-^2)}}$$