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Dissipative systems

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0. Introduction

A fundamental observation in nature is the irreversible time development of macroscopic systems. Such observations (in connection with the conversion from heat to mechanical work) led CLAUSIUS (1850) to the formulation of a variant of the second law of thermodynamics. CLAUSIUS made in 1865 a further important step: he showed on the basis of the second law the existence of a variable - the entropy S of the system, which is only a functional of the realized equilibrium state. The entropy S has for an isolated physical system the following property: is the system in an equilibrium state $\underline{p}$ and goes (because of changing the physical conditions) over into a new equilibrium state $\underline{q}$, then $S(\underline{p}) \leq S(\underline{q})$. In other words: for isolated systems the entropy never decreases and so indicates that a process $\underline{p} \rightarrow \underline{q}$ can not reversed if $S(\underline{p}) < S(\underline{q})$.

A dynamical description of such irreversible processes was possible only with the methods of statistical mechanics. The general idea is then the following: the irreversible temporal behaviour of physical systems is indicated by the monotone temporal behaviour of certain state functionals. The most famous example is the Boltzmann equation (as the evolution equation of the process) and the monotone behaviour of a state functional H - briefly H function (so called H theorem of Boltzmann, 1872).

In the following we speak about discrete, classical physical systems and introduce a family of state functionals. Then, we define a class of processes (called dissipative processes) by the claim that all this functionals show a monotone behaviour in time.

In a review we present some of the essential implications on the possible time developments of such dissipative systems.

1. Finite-dimensional classical systems

The <u>physical variables</u> of finite-dimensional systems are all vectors from R^n. This means: the components of $\underline{A} \in R^n$ give the possible values of the physical variable $\underline{A}$.
Then, a <u>state</u> (as a normalized element from the positive cone of the dual of R^n) is given by a n-dimensional probability vector $\underline{p}$: $\underline{p} = (p_1,\dots,p_n)$, $p_i \geqslant 0$ for all i and $\sum_i p_i = 1$. Accordingly a state is a expectation value functional for the physical variables:

$$\underline{A} \longrightarrow \langle \underline{A} \rangle_{\underline{p}} = \sum_i p_i A_i \ , \ \underline{A} \in R^n \ .$$

The set of all states (or all probability vectors) will be called the <u>state space</u> P_n. The interior of the state space is the set of the <u>strictly positive states</u> (i.e., all components of such a state $\underline{p}$ are positive - briefly $\underline{p} > \underline{0}$).
We describe the <u>time development</u> (or a process) of such a system by a trajectory in the state space P_n. I.e., we have a map[1], which determines a state $\underline{p}(t)$ for every instant of time t 0 ($\underline{p}(0)$ will be called the initial state).
Especially, we are interested in time developments which are given by a system of ordinary differential equations: $(d/dt)\, \underline{p} = \underline{v}(\underline{p})$
Differential equations will be called <u>P_n-invariant evolution equations</u>, when every solution which starts with initial value from the state space P_n can be extended to all times $t > 0$ and forever remains in P_n.
Now, we introduce state functionals. A fundamental notion is the discrete version of Boltzmann's H function /6/: $H(\underline{p}) = \sum_i p_i \log p_i$.

Let us consider the structure of $H(\underline{p})$. One notices easily that

$$H(\underline{p}) = \sum_i \left(\tfrac{1}{n}\right) \ g\left(p_i / (\tfrac{1}{n}) \right) - \log n \quad ,$$

when $g(s)$ represents the convex function s log s.
We generalize this expression in various aspects.
<u>Definition:</u> Let $g(s)$ be an arbitrary convex function (defined on R_+) and $\underline{p}$, $\underline{q}$ states ($\underline{q} > \underline{0}$).
Then we define <u>q-relative H functionals</u>

$$S_g(\underline{p}/\underline{q}) := \sum_i q_i \, g(p_i/q_i) \ .$$

We get Boltzmann's H (up to a constant) for the reference state $\underline{q} = (1/n, \ldots 1/n)$ and the convex function $g(s) = s \log s$.

Now, in connection with Boltzmann's H theorem we also formulate $\underline{q}$-relative H theorems.

Definition: A trajectory $(\underline{p}(t))_{t \geq 0}$ in the state space P_n fulfils the $\underline{q}$-relative H theorems if and only if for any convex function g

$$S_g(\underline{p}(t)/\underline{q}) \leq S_g(\underline{p}(t')/\underline{q})$$

when $t \geq t'$.

Remark 1. There is a nice geometric interpretation for processes which fulfil the $\underline{q}$-relative H theorems.

For a fixed state $\underline{q} > 0$ we define a partial order $\succ$ in P_n:
$/\underline{p}, \underline{q}/ \succ /\tilde{\underline{p}}, \underline{q}/$ ("$\underline{p}$ is relative to $\underline{q}$ more mixed than $\tilde{\underline{p}}$")

iff $S_g(\underline{p}/\underline{q}) \leq S_g(\tilde{\underline{p}}, \underline{q})$ for any convex g.

Equivalent definitions are the following ones (/1/)

(i) There exists a stochastic matrix A with
$A\tilde{\underline{p}} = \underline{p}$ and $A\underline{q} = \underline{q}$.

or

(ii) $//\underline{p} - \lambda \underline{q}//_1 \leq //\tilde{\underline{p}} - \lambda \underline{q}//_1$ for all $\lambda \in R_+$
$(//\underline{a}//_1 = \sum_i /a_i/, \ \underline{a} \in R^n)$

This shows the very regular behaviour of trajectories which fulfil relative H theorems: the state becomes more and more mixed (relative to the reference state) or (in other words) the distance functions (from (ii)) never increase. The dynamics is generated by stochastic transformations.

The introduced order relation is only a special case of a general relation between tupels and even n-tupels of vectors (see /1/). With the reference state $\underline{q} = (1/n, \ldots, 1/n)$ we get from the above defined relation a partial order which has been investigated already in classical works about matrix theory (SCHUR, OSTROWSKI, HARDY, LITTLEWOOD, POLYA and others). For the "non-commutative version" (with application in quantum mechanics founded by UHLMANN) see /2/ and also /8/.

Now, we illustrate the introduced concepts by an important example.

Remark 2. A fundamental equation in non-equilibrium statistical mechanics is the so called master equation:

$d/dt\ \underline{p} = L\underline{p}$ where L is a stochastic generator:

$L_{ii} \leq 0, \ L_{ik} \geq 0 \quad i \neq k, \quad \sum_i L_{ik} = 0$ for all k (i.e., a generator of a semi-group of stochastic matrices). One sees easily that such an equation can be written (possibly after rescaling of time) as a balance equation

$$\begin{aligned} d/dt\ p_i &= \sum_k (A_{ik}\, p_n - A_{ki}\, p_i) \\ &= (\sum_k A_{ik}\, p_k) - p_i \end{aligned} \qquad i = 1,\dots,n$$

with $A = (A_{ik})$ stochastic.

The physical interpretation is then the following: p_i determines the probability to find the system in the (pure) state $\underline{e}_i = (o,\dots,o,\underset{i}{1},o,\dots,o)$ and the A_{ik}'s give the probability per unit time for a transition from $\underline{e}_k$ to $\underline{e}_i$.

Because every solution $(\underline{p}(t))_{t\geq 0}$ is generated by a semi-group of stochastic matrices (which map states into states), master equations are P_n-invariant evolution equations. Further, we get immediately from Remark 1 (i) that all solutions of master equations (which start in P_n) fulfil the $\underline{q}$-relative H theorems with respect to every stationary state $\underline{q}$ (i.e. $L\underline{q} = \underline{o}$, $\underline{q} > \underline{0}$).

The direct proof is very simple. Is $t \geq t'$, then exists a stochastic matrix A with $\underline{p}(t) = A\,\underline{p}(t')$ $(A\underline{q} = \underline{q})$.

Now, $S_g(\underline{p}(t)/\underline{q}) = \sum_i q_i\, g\,(\frac{p_i}{q_i})$ $\qquad (\underline{p}(t') = (p_1',\dots))$

$$= \sum_i q_i\, g\,(\frac{\sum_k A_{ik}\, p_k'}{q_i}) = \sum_i q_i\, g\,(\sum_k \frac{A_{ik}\, q_k}{q_i} \cdot \frac{p_k'}{q_k})$$

$$\leq \sum_i q_i\,(\sum_k A_{ik}\frac{q_k}{q_i})\, g\,(\frac{p_k'}{q_k}) = S_g(\underline{p}(t')/\underline{q})$$

if we use that A is stochastic, $\underline{q}$ is fix-point of A and Jensen's inequality for convex functions.

PAULI introduced already 1928 a special master equation and proved a H theorem for Boltzmann's H functional. But the more general result was given only in 1940 by YOSIDA, obviously unnoticed and so many years later rediscovered.

2. Dissipative Processes

We call a process (in P_n) <u>dissipative</u>, when there exists a state $\underline{q}$ ($\underline{q} > 0$) such that the trajectory fulfils the $\underline{q}$-relative H theorems[2]. A <u>dissipative system</u> is a P_n-invariant evolution equation such that all solutions starting in P_n fulfil the $\underline{q}$-relative H theorems for the same state $\underline{q}$ ($\underline{q} > \underline{0}$).[2)]

Boltzmann used his H theorem to demonstrate (in an intuitive way) the asymptotic approach to the equilibrium state. What can we say about the asymptotic behaviour of dissipative processes or dissipative systems?

In general it is not valid that the trajectory of a dissipative process (with respect to $\underline{q}$) approaches $\underline{q}$ as $t \longrightarrow \infty$.

The general result is the following

Theorem 1. Let $(\underline{p}(t))_{t \geq 0}$ a (continuous) dissipative process (with respect to $\underline{q} > \underline{0}$).

Then, it exists $\lim_{t \to \infty} \underline{p}(t) = \underline{p}_\infty$. Further, let the initial state $\underline{p}(0) > \underline{0}$ than also $\underline{p}(t) > \underline{0}$ for all $t > 0$ and $\underline{p}_\infty > \underline{0}$.

In the case of dissipative systems we get

Theorem 2. Suppose we have a dissipative system (with respect to $\underline{q} > \underline{0}$) .

Then, every solution starting in P_n converges to a stationary state. Further, every solution starting in the interior of P_n remains there, and the asymptotic stationary state is also from the interior of P_n.

Which role plays the reference state $\underline{q}$?

Theorem 3. Suppose we have a dissipative system (with respect to $\underline{q} > \underline{0}$).

Then, $\underline{q}$ is a stationary state. If only finitely many strictly positive stationary states exist, then $\underline{q}$ is the only stable stationary state and asymptotically stable (stability in restriction to P_n).

Every solution starting with $\underline{p}(o) > \underline{0}$ approaches $\underline{q}$ as $t \to \infty$ if $\underline{q}$ is the only strictly positive stationary state.

Let us now give an impression of the proofs, which are given in /5/. We show a central fact: the convergence of the trajectories.

It is well-known from topological dynamics /7/ that the ω-limit set Ω [3)] of a trajectory in P_n (P_n is compact!) is a compact, nonvoid and connected set. Because of continuity of the trajectory and the H theorems, we get

$$S_g(\underline{p}/\underline{q}) = S_g(\underline{\tilde{p}}/\underline{q}) \quad \text{for all convex } g \text{ if } \underline{p}, \underline{\tilde{p}} \in \Omega .$$

Now we choose as special functionals the distance functions from chap. 1 (Remark 1 (ii)). Therefore, $\lambda \in R_+$

(+) $f(\lambda) = //\underline{p} - \lambda \underline{q}//_1$ is on Ω only a function of $\lambda \in R_+$

From this we conclude that Ω is a one-point set, because (+) shows that Ω has only finitely many elements, on the other hand: Ω is a non-void, connected set.

Some words about theorem 3. When we choose the reference state $\underline{q}$ as a initial state, then must be (for the distance function with $\lambda = 1$)

$$//\underline{q}(t) - \underline{q}//_1 \leq //\underline{q} - \underline{q}//_1 = 0 \quad \text{for all } t > 0$$

(because also the trajectory $\underline{q}(t)$ with $\underline{q}(0) = \underline{q}$ is dissipative).
From $//\underline{q}(t) - \underline{q}// = 0$ follows immediately the stationarity of $\underline{q}$: $\underline{q}(t) = \underline{q}$ for all $t \geqslant 0$.

Further, we can use some of the H functionals as Ljapunov functionals and investigate the stability properties of q.

3. Structure of dissipative systems

We already know an example of a dissipative system - the master equation. The class of all such systems contains however more complicated (nonlinear) systems.

Suppose we have a P_n-invariant evolution equation $(d/dt)\,\underline{p} = \underline{v}(\underline{p})$[4]. Which structure has the vectorfield $\underline{v}$ if we know that it is a dissipative systems?

<u>Theorem 4.</u> Let $(d/dt)\,\underline{p} = \underline{v}(\underline{p})$ be a P_n-invariant evolution equation.

We have a dissipative system (with respect to $\underline{q} > \underline{0}$) if and only if there exist a open, dense set $S \subset P_n$ and a map $L: S \ni \underline{p} \rightarrow L(\underline{p})$ from S into the real n×n-matrices with

(i) $L(\underline{p})$ is a stochastic generator

(ii) $L(\underline{p})\underline{q} = \underline{0}$

(iii) $\underline{v}(\underline{p}) = L(\underline{p})\underline{p}$ for all $\underline{p} \in S$.

The proof is in /5/. It uses concepts and arguments as explained in chap. 1 (Remark 1 and 2).

The theorem says that the vectorfield of a dissipative system is ("almost everywhere") given by a state-dependent stochastic generator $L(\underline{p})$. It is useful to compare the result with chap. 1 (Remark 2): the vectorfield of a master equation is given by a constant stochastic generator.

Our next aim is to investigate some often used systems: the quadratic systems. This means that the map L is affin on P_n

$$L(\underline{p}) = L(\textstyle\sum_k p_k \underline{e}_k) = \sum_k p_k L_k$$

with the stochastic generators $L(\underline{e}_k) = L_k$.

Such systems are P_n-invariant evolution equations (/5/). When even exists a state $\underline{q} > \underline{0}$ with $L_k\underline{q} = \underline{0}$ for all k, then we can apply theorem 4: the system is dissipative. Therefore we can also apply theorem 2 and 3.

If we suppose that $(\sum_k L_k)_{ij} \neq 0$ for all i, j, $\underline{q}$ is the only strictly positive stationary state of our system (this follows from the asymptotic properties of irreducible Markov chains /5/). In this case, $\underline{q}$ has the announced stability properties and is the asymptotic state for every trajectory.

We illustrate these facts by a second example. A differential equation of the following kind will be called Boltzmann-like equation (as a discrete caricature of the Boltzmann equation):

$$d/dt\ p_i = \sum_{j,k,l} (A_{ijkl}\ p_k p_l - A_{klij}\ p_i p_j) \qquad i = 1,\dots, n$$

with the properties for the scheme of the A_{ijkl}'s:

$$A_{ijkl} = A_{jikl} = A_{jilk} \geq 0 \quad \text{for all } i,j,k,l, \sum_{ij} A_{ijkl} = 1 \text{ for all } k,l$$

We define a sequence of stochastic nxn-matrices $B^{(k)}$:

$$B^{(k)}_{ij} = \sum_l A_{ilkj} \quad .$$

With this sequence $B^{(k)}$ we can write the vectorfield of Boltzmann-like equations

$$\underline{v}(\underline{p}) = (\sum_k p_k B^{(k)} - \underline{1})\underline{p} = (\sum_k p_k L_k)\underline{p} \quad \text{when } L_k = B^{(k)} - \underline{1},\ \underline{1} = (\delta_{ij}).$$

Now we are in position to formulate a corollary to our theorems.

Corollary. When we have a Boltzmann-like equation and we suppose that it exists a state $\underline{q} > \underline{0}$ with $L_k\underline{q} = \underline{0}$ for all k, i.e. $B^{(k)}\underline{q} = \underline{q}$ for all k, then we have a dissipative system (with respect to $\underline{q}$) and all solutions starting with $\underline{p}(0) > \underline{0}$ converges to $\underline{q}$ as $t \to \infty$.

The proof is obvious. We remark only: the property $B^{(k)}\underline{q} = \underline{q}$ garantees also that $(\sum_k L_k)_{ij} \neq 0$ for all i,j.

It is not difficult to give for every $\underline{q} > \underline{0}$ a scheme (A_{ijkl}) so that all conditions of the corollary are fulfilled (/3/).

We can interprete general Boltzmann-like equations as balance equations for collisions. p_i describes the probability to find a particle with property i, and A_{ijkl} gives the transition probability per unit time that a pair of particles with properties k,l is scattered into a pair with properties i,j.

In a similar way (if one uses theorem 4) every dissipative system can be interpreted as a balance equation with state-dependent transition probabilities.
The stated assertions are a contribution to the qualitative behaviour of this class of dynamical systems.
An additional class of "dissipative" systems is introduced and characterized in /4/.

1) We consider only continuous trajectories (at t = o from the right).

2) It can happen that more than one such state $\underline{q}$ exists!

3) I.e., the set of all limit points (in P_n) of the trajectory.

4) We suppose that the vectorfield $\underline{v}$ is continuously differentiable.

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