Order Structure (Majorization) and Irreversible Processes

Peter M. Alberti · Bernd Crell · Armin Uhlmann · Christian Zylka

1. The comparison of the information content of classical or quantum physical states leads to a partial order in the state space of the physical system. This partial order introduced by Uhlmann [68, 69, 71] has (for classical physical systems) well-known roots going back to Schur, Hardy, Littlewood, Polya, Karamata and others. We refer for a survey of these ideas and results (up to 1980) to Thirring [64, 65, 66], Wehrl [89] and the monographs by Alberti & Uhlmann [30, 34, 33].

2. In the following we will apply this partial order to the description of irreversible processes of classical physical systems with finite-dimensional state space and indicate some of the results. The state space $\mathbb{S}_n$ is the set of all probability vectors $\vec{p} = (p_1, p_2, \ldots, p_n)^T$ with $\sum_{i=1}^{n} p_i = 1$ and $p_i \geq 0$ for all i.
Let us start with the definition of the partial order for such systems[1]:

$$\vec{p} \prec \vec{q} \longleftrightarrow \text{There is a } \textit{doubly stochastic} \text{ matrix } T \text{ with } \quad \vec{p} = T\vec{q}.$$

An equivalent characterization is:

$$\vec{p} \prec \vec{q} \longleftrightarrow S_f(\vec{p}) \leq S_f(\vec{q}) \quad \text{for all convex functions f.}$$

The functionals $S_f(\cdot)$ are given by

$$S_f(\vec{p}) \underset{def}{=} \sum_{i=1}^{n} f(p_i).$$

Observe that we get a discrete version of the Boltzmann-Gibbs entropy if we choose $f(x) = x \log x$. Therefore the functionals $-S_f$ are called *generalized entropies* [2].

3. Now we extend this partial order to tuples of states. For this purpose let us consider two m-tuples $|\vec{p_1}, \vec{p_2}, \ldots \vec{p_m}|$ and $|\vec{q_1}, \vec{q_2}, \ldots \vec{q_m}|$ of states and define:

$$|\vec{p_1}, \vec{p_2}, \ldots \vec{p_m}| \prec |\vec{q_1}, \vec{q_2}, \ldots \vec{q_m}| \quad \longleftrightarrow$$

$$\text{There is a } \textit{stochastic} \text{ matrix } T \text{ with } \quad \vec{p_i} = T\vec{q_i} \quad \text{for all} \quad i = 1, \ldots m.$$

[1] This is just the partial order which is now well-known as *majorization*.
[2] Due to this fact "Uhlmann's school" defined these functionals originally with concave functions f and used the opposite sign for the order relation.

The stochastic matrix T transforms the states simultaneously. This partial order can also be characterized by convex functionals [9]:

$$|\vec{p_1}, \vec{p_2}, \dots \vec{p_m}| \prec |\vec{q_1}, \vec{q_2}, \dots \vec{q_m}| \quad \longleftrightarrow$$

$$S_g(\vec{p_1}, \vec{p_2}, \dots \vec{p_m}) \leq S_g(\vec{q_1}, \vec{q_2}, \dots \vec{q_m}) \text{ for all h-convex functions g.}$$

A function $g : \mathbb{R}^m \to \mathbb{R}$ is called h-convex, if it is simultaneously convex and homogeneous in all its arguments. The functional S_g is given by

$$S_g(\vec{p_1}, \vec{p_2}, \dots \vec{p_m}) \underset{def}{=} \sum_{i=1}^{n} g(p_{1i}, p_{2i}, \dots, p_{mi}),$$

where $\vec{p_k} = (p_{k1}, \dots, p_{kn}), k = 1, \dots, m$.
The case m = 2, i.e. pairs of states, is of particular interest. Using the homogeneity of the functions g let us write the functionals S_g for all states from the interior of the state space (i.e., only positive components) in the following way:

$$S_g(\vec{p_1}, \vec{p_2}) = \sum_{i=1}^{n} g(p_{1i}, p_{2i}) = \sum_{i=1}^{n} p_{2i} \cdot g(\frac{p_{1i}}{p_{2i}}, 1) = \sum_{i=1}^{n} p_{2i} \cdot f(\frac{p_{1i}}{p_{2i}})$$

with the convex function $f(x) = g(x, 1)$. Thus, it appears naturally to introduce

$$S_f(\vec{p_1}|\vec{p_2}) \underset{def}{=} \sum_{i=1}^{n} p_{2i} \cdot f(\frac{p_{1i}}{p_{2i}})$$

for all convex functions f. We will always use these functionals $S_f(\cdot|\cdot)$ if we consider pairs of states and call them *generalized relative entropies.* In particular, if we choose (as above) $f(x) = x \log x$ we get the relative entropy of the state $\vec{p_1}$ with respect to the state $\vec{p_2}$. The idea to extend the partial order to pairs of states is due to Mead and Ruch [58].

A special interest deserves the case that one of the states remains fixed. We choose a *reference state* $\vec{q}$ from the state space $\mathbb{S}_n$ and define a "relative" partial order (relative with respect to $\vec{q}$)

$$\vec{p_1} \underset{\vec{q}}{\prec} \vec{p_2} \longleftrightarrow |\vec{p_1}, \vec{q}| \prec |\vec{p_2}, \vec{q}|.$$

The relative partial order turns into our initial partial order in $\mathbb{S}_n$ if we choose the state $\vec{e} = (\frac{1}{n}, \frac{1}{n}, \dots, \frac{1}{n})$, the "equipartition", as reference state.

4. Next we study dynamical processes in the state space $\mathbb{S}_n$. Such processes can be represented by families of stochastic matrices.
It seems naturally to distinguish a class of processes which respects the partial order (with a fixed reference state $\vec{q}$ - which in this case is necessarily also a stationary state). In other words: Suppose $t \to \vec{p}(t)$ is any trajectory of our process, then

$$\vec{p}(t) \underset{\vec{q}}{\prec} \vec{p}(t') \text{ for all } t \geq t'.$$

This means in terms of the functionals $S_f(\cdot|\cdot)$ that the functions

$$t \to S_f(\vec{p}(t)|\vec{q})$$

decrease monotonously for *all* convex functions f.

Having in mind Boltzmanns and Paulis H theorems[3] from now on such processes are called *processes with $\vec{q}$-relative H theorems.* The study of processes with H theorems (relative to the "equipartition" $\vec{e}$) started with Laner/Laner [50] and Uhlmann [74]. An important step was the extension to arbitrary reference states by Ruch & Mead [58, 52], cf. also Uhlmann [75]).

Physically relevant irreversible processes with H theorems are already known for a longer time. Important examples are the so-called *master equations*

$$\frac{d}{dt}\vec{p} = L\vec{p},$$

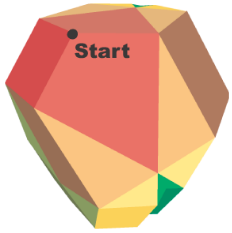
where the matrix $L = (L_{ik})$ is a generator of a semigroup of stochastic matrices and has therefore the following properties:

$$L_{ii} \leq 0, L_{ik} \geq 0 \text{ for } i \neq k, \sum_i L_{ik} = 0 \text{ for all } k.$$

It seems that in the classical papers by Yosida [94], Stueckelberg [63], Piron et al [46], Morimoto [53] and van Kampen [85] the H theorems are mentioned only incidentally. Maybe these H theorems were considered more or less as a special feature of linear (Markov) time developments. Examples of nonlinear evolution equations with H theorems are some families of Boltzmann-like equations (Wehrl & Yourgrau [91] und Crell & Uhlmann [40]), i.e., evolution equations in $\mathbb{S}_n$ with quadratic nonlinearities.

5. The systematic study of time evolutions (in state spaces) with H theorems began with the monographs by Alberti & Uhlmann[30], the papers by Alberti & Crell [21, 23], Kerstan [49] und Zylka [96, 97]. It turn out, that these time evolutions with H theorems have interesting geometrical features concerning the accessibility of states (Zylka [96, 97]) and allow for a lot of qualitative and quantitative results about the behavior of the solutions and the structure of the maps and vector fields, respectively, generating these evolutions (Alberti & Crell [21, 23, 24, 25]).
The sets of states which are accessible from a fixed initial state by processes with H theorems turns out to be non-convex polytopes (Zylka [97, 101]).

[3]These theorems describe the monotone behavior of the entropy for solutions of the Boltzmann equation [37] and Paulis master equation [56], respectively.



E.g., in the case $n = 4$, all trajectories starting from the red corner and fulfilling $t \to \vec{p}(t)$ with

$$\vec{p}(t) \underset{\vec{e}}{\prec} \vec{p}(t') \text{ for all } t \geq t'$$

will be trapped in the indicated polyhedron. In this context Zylka also studied some special families of matrices (generalized uniformly tapered, extremal majorizing, extremal anti-majorizing matrices)([47, 48]).
Furthermore Zylka gave some examples for physically relevant Schur-convex functionals, i.e., functionals that accompany the partial order monotonously. Especially there are examples of Schur-convex partitions functions that appear in statistical mechanics (Zylka et al [102, 103]).

Let us formulate some of the results. We start with a structure theorem for vector fields generating time evolutions with H theorems[4]:

The evolution equation

$$\frac{d}{dt}\vec{p} = L(\vec{p})\,\vec{p}$$

generate a process with $\vec{q}$-relative H theorems in $\mathbb{S}_n$ *if and only if*

1. $L(\vec{p})$ is for every $\vec{p} \in \mathbb{S}_n$ a generator of a semigroup of stochastic matrices, i.e.,
$$L_{ii}(\vec{p}) \leq 0,\, L_{ik}(\vec{p}) \geq 0 \text{ for } i \neq k,\, \sum_i L_{ik}(\vec{p}) = 0 \text{ for all } k$$
2. $L(\vec{p})\,\vec{q} = 0$ for all $\vec{p} \in \mathbb{S}_n$.

These vector fields generate indeed an evolution in the state space whose solutions always converge asymptotically to a stationary state. This stationary state is not necessarily the reference state. Criteria for the stability of the stationary states, for ergodic properties, and detailed results on the velocity of convergence are known. We get some refinements for evolution equations with quadratic nonlinearities (Boltzmann-like equations). These equations describe balances in "collision-like processes" and have a lot of applications. In this case the vector field $L(\vec{p})$ has the structure

$$L(\vec{p}) = \sum_i p_i \cdot L^i,$$

[4]In order to avoid technical details we consider only continuously differentiable vector fields.

where all L^i are generators of semigroups of stochastic matrices. Using $L^i = (L^i_{jk})$ we obtain for the Boltzmann-like equations

$$\frac{d}{dt}p_j = \sum_{j,k=1}^{n} L^i_{jk}\, p_i p_k \;,\; j = 1, \ldots n.$$

Non-linear evolution equations whose solutions are always solutions of a (solution-dependent!) master equation were investigated, too. Alberti & Crell proved [22] that this property is connected with conservation quantities which enforce a foliation of the state space.

An interesting characterization of the solutions of master equations was obtained by Alberti und Uhlmann [31, 32] by means of the partial order.
Let $t \to \vec{p}\,(t)$ be the trajectory of a master equation

$$\frac{d}{dt}\vec{p} = L\vec{p},$$

then holds evidently for every m $(m = 1, 2, \ldots)$, arbitrary times $t_1, \ldots, t_m$ and arbitrary $s > 0$,

$$|\vec{p}\,(t_1 + s), \ldots, \vec{p}\,(t_m + s)| \;\prec\; |\vec{p}\,(t_1), \ldots, \vec{p}\,(t_m)|.$$

But the converse is also true:

A trajectory $t \to \vec{p}(t)$ showing this order for every m $(m = 1, 2, \ldots)$, arbitrary times $t_1, \ldots, t_m$ and arbitrary time shift $s > 0$ is a solution of a master equation.

Thanks to Peter Serocka (Bielefeld) for his help with the graphics.

The following bibliography contains some further references on the subject.

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E-mail addresses:
alberti@fh-erfurt.de
bernd.crell@itp.uni-leipzig.de
armin.uhlmann@itp.uni-leipzig.de
zylka@fh-erfurt.de