On the statistical viewpoint concerning the second law of thermodynamics
- a reminder on the Ehrenfests’ urn model -

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Abstract
In statistical thermodynamics the 2nd law is properly spelled out in terms of conditioned probabilities. As such it makes the statement that “entropy increases with time” without preferring a time direction. In this paper we wish to explain and illustrate this statement in terms of the Ehrenfests’ urn model in a way that hopefully adds some clarifying aspects concerning the role of time-conditioned probabilities. We will relate past- and future-conditioned probabilities through Bayes’ rule, which allows us to explicitly state what is meant by time-reversal invariance in this context.

This paper is my contribution to the book From Quantum to Classical – Essays in Honour of H.-Dieter Zeh, edited by Claus Kiefer, that appeared in 2022 as volume 204 in the series Fundamental Theories of Physics at Springer Verlag.

1 Prologue
This contribution is dedicated to the memory of H. Dieter Zeh, with whom I had many discussions over a period of time that easily spans a quarter of a century. These discussions were usually controversial, sometimes very controversial, so that often we could only agree do disagree. From these discussions I learned a lot!

I came to know Zeh - the university teacher - in my earlier student days. In June 1984 a friend gave me Zeh’s “Die Physik der Zeitrichtung” as a birthday present [Zeh, 1984]. Below the preface my friend wrote in his own hand: “I am sure this book will find your undivided approval”, and it did! Not so much because I felt competent enough to judge the content, but because I felt a degree of veracity behind it that appealed to me very much.

The book of which I received a copy was the first edition, based on notes of lectures Zeh had given since 1979. When the first edition finally came out it quickly circulated amongst the younger generation of students, even outside the physics department (in fact, my friend was in the department of chemistry and knew about the book before I did). For many of us Zeh represented the serious
and uncompromising urge for real “understanding” that many of us hoped to find at the university and, in particular, in the department of theoretical physics. This hope was not always fulfilled but Zeh was definitely someone proving that our hopes had not been in vain.

I should add that our trust was based not so much on the fact that Zeh talked about the “big issues”, like “arrow of time”, or “interpretation of quantum mechanics”, which clearly fascinate all beginning student alike, but rather on the fact that he touched upon these issues while at the same time striving for full clarity as regards the “small issues”. The only lecture I took by Zeh was on analytical mechanics. From that I remember his explanation of the Euler angles, which he gave by means of meticulous blackboard drawing that he had prepared before the lecture, showing four systems of orthonormal frames in different colours with the relevant rotation axes and angles. His comment was that he did not understand the corresponding drawing in the standard textbook then widely used, so he developed everything from scratch again.

Many years later Zeh gave me the third English edition (Zeh, 1999) as a present. That edition contains a new Appendix on a simple numerical toy model, the so called ring model, taken from Kac (1959, chapter 3), which is meant to illustrate the concept of a “Zwanzig projection”, that plays a most central role in Zeh’s book, as one can already see from the book’s bibliography, that contains 43 entries for that term (the only entry under “Z”). Zeh also mentions the Ehrenfest’s urn-model as a popular and widely known one to illustrate conceptual points connected with statistical statements in physics. I remember discussing that with Zeh and that I praised the Ehrenfests’ model for its ability to illustrate basic but non-trivial concepts from statistical mechanics by means of exact mathematical expressions. It was then that I worked out some details of that model, just for my own understanding, illustrating – as Zeh used to say – the “fact-like” rather than “law-like” nature of entropy increase. This is what I wish to present here.

Following the third, there were two more editions of Zeh’s classic text, the last (fifth) in Springer’s Frontiers Collection (Zeh, 2007), that I reviewed in Giulini (2008).

2 Introduction

The point that the likely statistical increase of entropy does not as such prefer a direction of time has been first made by Ehrenfest (1907) in connection with their urn model (Ehrenfest, 1906); see also their general review Ehrenfest (1912) (English translation Ehrenfest and Ehrenfest (1990)). It has again been emphasised by von Weizsäcker (1939). This insight is not new and should be

\footnote{To give a contrasting example, I remember from my first lecture on quantum field theory, in which after the scheme of canonical quantisation was introduced and the interaction picture mentioned, the professor said: “There is a theorem due to Rudolf Haag, according to which the interaction picture does not exist; but we shall henceforth ignore that!” How should a serious beginning student deal with such a casually tossed comment?}

\footnote{The conclusions Weizsäcker drew from this insight are, however, problematic; see Kiefer (2014)}
a commonplace, though that is far from true according to my experience.

Without going into any analytical details, Zeh said it very clearly at the beginning of paragraph 3 of Zeh (2007, p 40) on the thermodynamical arrow of time:

“While statistical considerations are indeed essential for the understanding of thermodynamical concepts, statistics as a method of counting has nothing a priori to do with dynamics. Therefore, it cannot by itself explain dynamically ‘irreversible’ processes – characterized by \(\{dS/dt\}_{\text{int}} > 0\). This requires additional assumptions, which often remain unnoticed, since they appear ‘natural’ to our prejudiced way of thinking in terms of causes (exclusively in the past). These hidden assumptions have therefore to be carefully investigated in order to reveal the true origin of the thermodynamical arrow.”

Zeh continues by comparing the four possibilities of processes in time

\[
\text{probable / improbale state } \xrightarrow{t} \text{ probable / improbable state}
\]

pointing out, in particular, that there are as many processes from improbable to probable than from probable to improbable states. Hence, an asymmetry in their number of occurrences must be connected with an additional, symmetry breaking assumption of an improbable state at one end of the time axis. Zeh calls that prescribed state the “initial” one, which at this point may be read as an implicit definition of “initial”, namely as that end at which the condition is put, for otherwise there is so far no objective difference between the two ends of the time axis.

In this contribution I will employ the celebrated urn model to exemplify these points. This model has once even been called “probably one of the most instructive models in the whole of physics” Kac (1959, p 73). The rather simple analytical features of this model help to guide one’s own expectations and reduce the danger of possible misconceptions. For the issue to be discussed here, namely that of the “likely increase” of entropy is a time symmetric statement, possible misconceptions have to do with a failure to appreciate the fact that the probabilities are conditioned in time, and that their interpretation, namely as being either “retarded” or “advanced”, is in itself indistinguishable unless a time orientation has already been established.

I will proceed as follows: In the next section I will try to put the qualitative statement just made into more precise words. In the following section this is then quantitatively analysed in terms of the urn model, where probabilities can actually be calculated in an explicit and elementary way. The remaining sections then discuss Boltzmann entropy, Gibbs entropy and H-theorem, and

3In the first (german) edition and in the following english editions up to, and including, the third, the “has nothing a priori to do with dynamics” reads instead: “has nothing a priori to do with the physical concept of time or its direction” Zeh (1992, p 37), or “...jedoch hat die Statistik als mathematische Disziplin nichts mit der physikalischen Zeit zu tun und vermag daher den Zeitrufel auch nicht zu begründen” Zeh (1984, p 23).
the thermodynamic limit and deterministic dynamics. Some elementary notions from probability theory that we made freely use of are collected in a short appendix.

3 The basic statements

In this section we start by making some of the previous statements more precise. We think of an idealised system, whose state may only change at sharp, discrete times. This allows us to speak unambiguously about “next” and “previous” points in time. Now we make the following

Assumption. At time $t_i$ the system is in a state $z(t_i)$ of non-maximal entropy. The statistical 2nd law now makes the following statement about conditioned probabilities (the condition, which is just this assumption, will not be repeated):

**Statement 1.** The probability, that the state $z(t_i)$ will develop in the future to a state $z(t_{i+1})$ of larger entropy, is larger than the probability for a development into a state of smaller entropy.

**Statement 2.** The probability, that the state $z(t_i)$ has developed in the past from a state $z(t_{i-1})$ of larger entropy, is larger than the probability of a development from a state of smaller entropy.

**Consequence 3.** The likely increase of entropy in the future state-development $z(t_i) \mapsto z(t_{i+1})$ does not imply a likely decrease for the (fictitious) past development $z(t_i) \mapsto z(t_{i-1})$, but rather also a likely increase.

**Consequence 4.** The most likely development $z(t_{i-1}) \mapsto z(t_i)$ is that of decreasing entropy. Somewhat ironically, one may say that it is more likely for the state $z(t_i)$ to come about through the improbable development from a more probable state $z(t_{i-1})$ than through the probable development from an improbable state.

To properly understand the last consequence, recall that our condition is placed on $z(t_i)$, that is at time $t_i$. For $z(t_i) \mapsto z(t_{i+1})$ this means a retarded or initial condition, for $z(t_{i-1}) \mapsto z(t_i)$, however, an advanced or final condition. It is this change of condition which makes this behaviour of entropy possible.

**Consequence 5.** The mere (likely) increase of entropy does not provide an orientation of time. It does not serve to define a ‘thermodynamic arrow of time’. Rather, an orientation is usually given by considering a definite time-interval (usually of finite length) and imposing a low-entropy condition at one of the two ends of that interval. Without further structural elements that would serve to distinguish the two ends, the apparently existing two possibilities to place the low-entropy conditions are, in fact, identical. An apparent distinction is sometimes introduced by stating that the condition at one end is to be understood as initial. But at this level this merely defines initial to be used for that very end at which the condition is placed.
4 The Urn-Model

This model was introduced by Ehrenfest (1906, 1907) and quickly entered textbooks and other pedagogical oriented discussions. More detailed mathematical discussion of it are contained in Kohlrausch and Schrödinger (1926), reprinted in Schrödinger (1984, pp. 349-357) and Kac (1947, 1959). Kohlrausch and Schrödinger (1926) also report on actual experiments done in order to determine the Boltzmann H-curve for this model.

Think of two urns, $U_0$ and $U_1$, among which one distributes $N$ numbered balls. For exact equipartition to be possible we assume $N$ to be even. A microstate is given by the individual numbers (names) of balls contained in $U_1$. (The complementary set of numbers then label the balls in $U_0$.) To formalise this, we associate a two-valued quantity $x_i \in \{0, 1\}$, $i \in \{1, \ldots, N\}$, to each ball, where $x_i = 0$ ($x_i = 1$) stands for the $i$'th ball being in $U_0$ ($U_1$). This identifies the set of microstates, which we will call $\Gamma$ (it corresponds to phase space), with $\Gamma = \{0, 1\}^N$, a discrete space of of $2^N$ elements. It can be further identified with the set of all functions $\{1, \cdots, N\} \to \{0, 1\}$, $i \mapsto x_i$. Mathematically speaking, the space $\Gamma$ carries a natural measure, $\mu_r$, given by associating to each subset $\Lambda \subset \Gamma$ its cardinality: $\mu_r(\Lambda) = |\Lambda|$. We now make the physical assumption, that the probability measure (normalized measure) $\nu_r := 2^{-N}\mu_r$ gives the correct physical probabilities. Note that this is a statement about the dynamics, which here my be expressed by saying, that in the course of the dynamics of the system, all microstates are reached equally often on time average.

Physical observables correspond to functions $\Gamma \to \mathbb{R}$. We call the set of such functions $\mathcal{O}$. Conversely, it is generally impossible to associate a physically realisable observable to any element in $\mathcal{O}$. Let $\{O_1, \ldots, O_n\} =: O_{re} \subset \mathcal{O}$ be the physically realisable ones, which we can combine into a single $n$-component observable $O_{re} \in \mathcal{O}^n$. If $O_{re} : \Gamma \to \mathbb{R}^n$ is injective, the state is determined by the value of $O_{re}$. In case of thermodynamical systems it is essential to be far away from injectivity, in the sense that a given value $\alpha \in \mathbb{R}^n$ should have a sufficiently large pre-image $O_{re}^{-1}(\alpha) \subset \Gamma$. The coarse-grained of macroscopic state space is then given by the image $\Omega \subset \mathbb{R}^n$ of the realized observables $O_{re}$. To every macrostate $\alpha \in \Omega$ corresponds a set of microstates: $\Gamma_{\alpha} := O_{re}^{-1}(\alpha) \subset \Gamma$. The latter form a partition of $\Gamma$: $\Gamma_{\alpha} \cap \Gamma_{\beta} = \emptyset$ if $\alpha \neq \beta$ and $\bigcup_{\alpha \in \Omega} \Gamma_{\alpha} = \Gamma$.

The realised observable for the urn-model is given by the number of balls in $U_1$, that is, $O_{re} = \sum_{i=1}^N x_i$. Its range is the set $\Omega = \{0, 1, \ldots, N\}$ of macrostates, which contains $N + 1$ elements. The macrostates are denoted by $z$. To $z$ there corresponds the set $\Gamma_z$ of $\binom{N}{z}$ microstates. The probability measure $\nu_r$ induces so-called ‘a-priori-probabilities’ for macrostates $z$:

$$W_{ap}(z) = \nu_r(\Gamma_z) = 2^{-N} \binom{N}{z}. \quad (1)$$

Let $X : \Omega \to \mathbb{R}$ be the random variable $z \mapsto X(z) = z$. Its expectation value, denoted by $E$, and its standard deviation, denoted by $S$, with respect to the

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4The subscript ‘re’ can be read as abbreviation for ‘realised’ or ‘relevant’.
a-priori-distribution \( \Pi \) are given by

\[
E(X, ap) = \frac{N}{2}, \quad S(X, ap) = \frac{\sqrt{N}}{2}.
\]

This follows from

\[
E(X; ap) = 2^{-N} \sum_{z=1}^{N} z \binom{N}{z} = 2^{-N} N \sum_{m=0}^{N-1} \binom{N-1}{m} = \frac{N}{2},
\]

\[
E(X^2 - X; ap) = 2^{-N} \sum_{z=2}^{N} z(z-1) \binom{N}{z} = 2^{-N} N(N-1) \sum_{m=0}^{N-2} \binom{N-2}{m} = \frac{N(N-1)}{4},
\]

\[
S^2(X; ap) = E(X^2 - X; ap) + E(X; ap) - E^2(X; ap).
\]

The system has a Markovian random evolution, which is defined as follows: At every time \( t_i \), where \( i = \{0,1,2,\ldots\} \) with \( t_j > t_i \) for \( j > i \), a random generator picks a number \( n \) in the interval \( 1 \leq n \leq N \). Subsequently the ball with number \( n \) changes the urn. There are two possibilities: The ball with number \( n \) has been in urn \( U_0 \) so that the change of macrostate is given by \( z \rightarrow z + 1 \). Alternatively, the ball has been in \( U_1 \) and the change of macrostate is given by \( z \rightarrow z - 1 \). The conditional probabilities, \( W(z \pm 1; t_{i+1}|z; t_i) \), that given the state \( z \) at time \( t_i \) the evolution will yield the state \( z \pm 1 \) at time \( t_{i+1} \), are given by

\[
W(z + 1; t_{i+1}|z; t_i) = \frac{N - z}{N} =: W_{\text{ret}}(z + 1|z),
\]

\[
W(z - 1; t_{i+1}|z; t_i) = \frac{z}{N} =: W_{\text{ret}}(z - 1|z).
\]

Since these are independent of time, we can suppress the arguments \( t_i \). We just have to keep in mind that the left entry, \( z \pm 1 \), is one time step after the time of \( z \), that is, the probabilities are past-conditioned or retarded. We indicate this by writing \( W_{\text{ret}} \).

Let \( W(z; t_i) \) denote some chosen absolute probability for the state to be \( z \) at time \( t_i \) and \( W_i : z \rightarrow W(z; t_i) \) the probability distribution at time \( t_i \). The dynamics described above will now induce a dynamical law, \( W_i \rightarrow W_{i+1}, \) on such distributions, given by

\[
W(z; t_{i+1}) = W(z; t_{i+1}|z + 1; t_i) W(z + 1; t_i) + W(z; t_{i+1}|z - 1; t_i) W(z - 1; t_i)
\]

\[
= \frac{z + 1}{N} W(z + 1; t_i) + \frac{N - z + 1}{N} W(z - 1; t_i),
\]

whose Markovian character is obvious. To be sure, \( W_i, i > 0, \) will depend on the initial distribution \( W_0 \). This dependence will be essential if \( W_0 \) is far from
equilibrium and the number of time steps \( i \) not much larger than the number \( N \) of balls. Conversely, one expects that for \( W_i \) will approach an equilibrium distribution \( W_{\text{stat}} \) for \( i \gg N \), where \( W_{\text{stat}} \) is independent of \( W_0 \). Its uniqueness is shown by

**Theorem 6.** A distribution \( W_{\text{stat}} \) which is stationary under \( \{\mathcal{A}\} \) is uniquely given by \( W_{\text{ap}} \) in (1).

**Proof.** We show, that \( W_{\text{stat}} \) can be uniquely determined from \( \{\mathcal{A}\} \). To this end, we assume a time independent distribution \( W_{\text{stat}} \) and write \( \{\mathcal{A}\} \) in the form

\[
W_{\text{stat}}(z+1) = \frac{N}{z+1} W_{\text{stat}}(z) - \frac{N - z + 1}{z+1} W_{\text{stat}}(z-1). \tag{9}
\]

Since \( W_{\text{stat}}(-1) = 0 \) we have for \( z = 0 \) that \( W_{\text{stat}}(1) = NW_{\text{stat}}(0) \), hence recursively \( W_{\text{stat}}(2) = \frac{1}{2} N(N-1) W_{\text{stat}}(0) \) and \( W_{\text{stat}}(3) = \frac{1}{6} N(N-1)(N-2) W_{\text{stat}}(0) \). By induction we get the general formula \( W_{\text{stat}}(z) = \binom{N}{z} W_{\text{stat}}(0) \). Indeed, inserting this expression for \( z \) and \( z-1 \) into the right hand side of (7), we obtain

\[
W_{\text{stat}}(z+1) = \left[ \frac{N}{z+1} \binom{N}{z} - \frac{N - z + 1}{z+1} \binom{N}{z-1} \right] W_{\text{stat}}(0) \\
= (N-z) \frac{N(N-1) \cdots (N-z+1)}{(z+1)!} W_{\text{stat}}(0) \\
= \binom{N}{z+1} W_{\text{stat}}(0). \tag{10}
\]

The value of \( W_{\text{stat}}(0) \) is finally determined by the normalization condition:

\[
1 = \sum_{z=0}^{N} W_{\text{stat}}(z) = W_{\text{stat}}(0) \sum_{z=0}^{N} \binom{N}{z} = W_{\text{stat}}(0) 2^N \Rightarrow W_{\text{stat}}(0) = 2^{-N}. \tag{11}
\]

**4.1 Future-conditioned probabilities and Bayes’ rule**

Consider a probability space and a set of events, \( \{A_1, \ldots, A_n\} \), which is 1.) complete, i.e. \( A_1 \cup \cdots \cup A_n = 1 \) (here 1 denotes the certain event), and 2.) mutually exclusive, i.e. \( i \neq j \Rightarrow A_i \cap A_j = 0 \) (here 0 denotes the impossible event). The probability of an event \( B \) then obeys the well known rule

\[
W(B) = \sum_{k=1}^{n} W(B|A_k) W(A_k).
\]

This is just what we used in (7). Now, Bayes’ rule, which we here regard as an independent assumption, will now allow us to deduce the inversely conditioned probabilities:

\[
W(A_k|B) = \frac{W(B|A_k) W(A_k)}{\sum_{l=1}^{n} W(B|A_l) W(A_l)}.
\tag{12}
\]

We now identify the \( A_i \) with the \( N+1 \) events \( \{z'; t_i\} \) at the fixed time \( t_i \), where \( z' = 0, \ldots, N \), and \( A_k \) with the special event \( \{z I; t_i\} \). Further we identify the

\footnote{Therefore we avoid to call it Bayes’ theorem.}
event \( B \) with \((z; t_{i+1})\), i.e. with the occurrence of \( z \) at the later time \( t_{i+1} \). Then we obtain:

\[
W(z \pm 1; t_i | z; t_{i+1}) = \frac{W(z; t_{i+1} | z \pm 1; t_i)W(z \pm 1; t_i)}{\sum_{z' = 0}^N W(z; t_{i+1} | z'; t_i)W(z'; t_i)}
\]

(13)

\[
= \frac{W(z; t_{i+1} | z \pm 1; t_i)W(z \pm 1; t_i)}{W(z; t_{i+1})}. \tag{14}
\]

Hence, given \( W_i \), a formal application of Bayes’ rule allows us to express the future conditioned (‘advanced’) probabilities in terms of the past conditioned (‘retarded’) ones. In our case we think of the latter ones as given by \((5-6)\). Hence we obtain the conditioned probability for \((z \pm 1; t_i)\), given that at the later time \( t_{i+1} \) the state will \( z \) occur:

\[
W(z + 1; t_i | z; t_{i+1}) = \frac{W(z + 1; t_i)}{W(z + 1; t_i) + \frac{N - z + 1}{z + 1}W(z - 1; t_i)}, \tag{15}
\]

\[
W(z - 1; t_i | z; t_{i+1}) = \frac{W(z - 1; t_i)}{W(z - 1; t_i) + \frac{z + 1}{N - z + 1}W(z + 1; t_i)}. \tag{16}
\]

### 4.2 Flow equilibrium

The condition for having flow equilibrium for the pair of times \( t_i, t_{i+1} \) reads

\[
W(z \pm 1; t_{i+1} | z; t_i)W(z; t_i) = W(z; t_{i+1} | z \pm 1; t_i)W(z \pm 1; t_i). \tag{17}
\]

It already implies \( W_i = W_{ap} \), since \((5-6)\) give \( W(z + 1; t_i) = \frac{N - z + 1}{z + 1}W(z; t_i) \) which leads to \( W(z; t_i) = \left(\frac{N}{z}\right)W(0; t_i) \). Since \( 1 = \sum_z W(z; t_i) \) we have \( W(0; t_i) = 2^{-N} \). Using Theorem 1, we conclude that flow equilibrium at \( t_i \) implies \( W_j = W_{ap} \) for \( j \geq i \).

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\( ^6 \)Without using \((5-6)\) one gets

\[
W(z \pm 1; t_{i+1} | z; t_i)W(z; t_i) = W(z; t_{i+1} | z \pm 1; t_i)W(z \pm 1; t_i) = W(z \pm 1; t_i | z; t_{i+1})W(z; t_{i+1}), \tag{18}
\]

where the last equality is the identity \( W(a|b)W(b) = W(b|a)W(a) \). The local (in time) condition of flow equilibrium is therefore equivalent to \((19)\)

\[
\frac{W(z \pm 1; t_{i+1} | z; t_i)}{W(z \pm 1; t_i | z; t_{i+1})} = \frac{W(z; t_{i+1})}{W(z; t_i)}. \tag{19}
\]
4.3 Time-reversal invariance

To be distinguished from flow equilibrium is time-reversal invariance. The latter is given by the following equality of past- and future-conditioned probabilities:

\[
W(z \pm 1; t_{i+1}|z; t_i) = W(z \pm 1; t_i|z; t_{i+1}) \quad (20)
\]

\[
W(z; t_{i+1}|z \pm 1; t_i) \frac{W(z \pm 1; t_i)}{W(z; t_{i+1})}, \quad (21)
\]

\[
W(z; t_{i+1}) = \frac{z + 1}{\binom{N}{2} N - z} W(z + 1; t_i) \quad (22)
\]

\[
= \frac{N - z + 1}{z} W(z - 1; t_i). \quad (23)
\]

It is interesting to note that the condition of time-reversal invariance is weaker than that of flow equilibrium. The former is implied by, but does not itself imply, the equilibrium distribution. Let us explain this in more detail: Equations \((22)\) and \((23)\) imply \((8)\), since \(\frac{N - z}{\binom{N}{2} N - z} \times (22) + \frac{1}{\binom{N}{2}} \times (23) = (8)\). Hence \((22)\) and \((23)\) are stable under time evolution \((8)\). Conversely, \((22)\) and \((23)\) is implied by \((8)\) and the following equation, expressing the equality of the right hand sides of \((22)\) and \((23)\):

\[
W(z + 1; t_i) = \frac{N - z}{z} \frac{N - z + 1}{z} W(z - 1; t_i).
\]

(24)

Indeed, eliminating \(W(z + 1; t_i)\) in \((8)\) using \((24)\), one gets

\[
W(z; t_{i+1}) = \frac{N - z + 1}{z} W(z - 1; t_i) \quad (25)
\]

hence \((22)\) and \((23)\). Time-reversal invariance for future times is therefore equivalent to the ‘constraint’ \((24)\) for the initial condition. It allows for a one-parameter family of solutions, since it determines \(W_i\) for given \(p := W(0; t_i)\) and \(q := W(1; t_i)\). Indeed, in analogy to the proof of Theorem 1 one gets \(W_i(z) = p \left( \frac{N}{z} \right)\)

for \(z\) even and \(W_i(z) = p \left( \frac{N}{z} \right)\) for \(z\) odd. Since \(\sum_{z=\text{even}} \binom{N}{z} = \sum_{z=\text{odd}} \binom{N}{z} = 2^{N-1}\), the normalization condition leads to \(1 = 2^{N-1}(p + \frac{N}{N-1}) \Rightarrow q = N(2^{-(N-1)} - p)\). This shows that \(p \in [0, 2^{-(N-1)}]\) faithfully parameterizes all distributions obeying \((24)\). One should note that solutions to \((24)\) are closed under convex sums. In this way one sees, that the obtained distributions are the convex sum

\(W_i = pW^e + (1-p)W^o\) of the ‘even’ distribution, \(W^e(z) = (1-(1)^{z-1})2^{-N} \left( \frac{N}{z} \right)\)

and ‘odd’ distribution, \(W^o(z) = (1-(1)^{z-1})2^{-N} \left( \frac{N}{z} \right)\). Solutions to \((24)\) form a closed interval within the simplex \(\Delta^N\), which connects the point \(W^e\) in the \(\frac{N}{2}\) sub-simplex \(\Delta_{13 \ldots N-1}\) with the point \(W^o\) on the \((\frac{N}{2} + 1)\)-sub-simplex \(\Delta_{34 \ldots N}\).

If we call this interval \(\Delta\), we have

**Theorem 7.** The set \(\Delta^* \subset \mathcal{W}\) is invariant under time evolution. The future development using \(W(z; t_{i+1}|z'; t_i)\) and the past development using \(W(z; t_i|z'; t_{i+1})\)
It is of central importance to note that the past development is, mathematically speaking, not the inverse operation to the future development. The reason being precisely that such a change in the direction of development is linked with a change from retarded to advanced conditionings in the probabilities.

5 General Consequences

In the following we want to restrict to the equilibrium condition. In this case the future-conditioned probabilities are independent of the \( t_i \) and we can write:

\[
W(z \pm 1; t_i | z; t_{i+1}) =: W_{av}(z \pm 1 | z).
\]

Hence we have:

\[
W_{ret}(z + 1 | z) = W_{av}(z + 1 | z) = \frac{N - z}{N}, \quad (28)
\]

\[
W_{ret}(z - 1 | z) = W_{av}(z - 1 | z) = \frac{z}{N}, \quad (29)
\]

from which statements 1 and 2 made in the Introduction follow. Indeed, let \( z = z(t_i) > N/2 \), then the probabilities that at time \( t_{i-1} \) or \( t_{i+1} \) the state was or will be \( z - 1 \) is, in both cases, given by \( \frac{N - z}{N} \). The probability for the state \( z + 1 \) at time \( t_{i-1} \) or \( t_{i+1} \) is \( \frac{N - z}{N} \). Now, every change of state in the direction of the equilibrium distribution leads to an increase in entropy (see below). Hence the probability of having a higher entropy at \( t_{i-1} \) or \( t_{i+1} \) is \( \frac{z}{N - z} \) times that of having a lower entropy. If \( z = z(t_i) < N/2 \) we have to use the inverse of that.

5.1 Boltzmann Entropy

Boltzmann Entropy \( S_B \) is a function \( S_B : \Omega \rightarrow \mathbb{R} \). We stress that since \( \Omega \) is defined only after a choice of coarse graining (i.e. a choice of \( \mathcal{O}_{re} \)) has been

\footnote{Explicitly one can see the preservation of (24) under time evolution (8) as follows: Given that the initial distribution \( W_i \) satisfies (24), the development (8) is equivalent to (22-23). Hence}

\[
W(z - 1; t_i) = \frac{z}{N - z + 1} W(z; t_{i+1}) \quad (26)
\]

\[
W(z + 1; t_i) = \frac{z + 2}{N - z - 1} W(z + 2; t_{i+1}) \quad (27)
\]

which allows to rewrite (24) for \( W_i \) into (24) for \( W_{i+1} \).
made, Boltzmann Entropy, too, must be understood as relative to that choice.

The value $S_B(z)$ in the macrostate $z$ is defined by $S_B(z) := \ln \mu_r(\Gamma_z)$. For the urn model this corresponds to the logarithm of microstates that correspond to the macrostate $z$. In what follows it will sometimes be more convenient to label the macrostate not by $z \in [0, N]$, but rather by a parameter $\sigma \in [-1, 1]$ of range independent of $N$. Let the latter be defined by $z = \frac{N}{2}(1 + \sigma)$. If we assume that $N, z, (N - z) \gg 1$ and approximate $\ln N! = N \ln N - N + O(\ln N)$ (Stirling formula), we obtain the following expression for the Boltzmann entropy:

\[ S_B(z) = N \ln N - z \ln z - (N - z) \ln (N - z), \quad (30) \]

\[ S_B(\sigma) = -\frac{N}{2} \left[ \ln \frac{1 - \sigma^2}{4} + \sigma \ln \frac{1 + \sigma}{1 - \sigma} \right]. \quad (31) \]

It obeys $S_B(\sigma) = S_B(-\sigma) = S_B(|\sigma|)$, which just corresponds to the invariance of the first expression under $z \mapsto N - z$. Considered as function of $|\sigma|$, $S_B : [0, 1] \rightarrow [\ln 2^N, 0]$ is strictly monotonically decreasing. That $S_B(\sigma = 1) = 0$ is best seen in the limit $z \rightarrow N$ of (30). Despite Stirling’s approximation this value is, in fact, exact, as one easily infers from the fact that $z = N$ just corresponds to a single microstate. In contrast, the given value at $\sigma = 0$ is only approximately valid.

### 5.2 Consequences 1 and 2

The quantitative form of Consequences 1 and 2 are given by the solution to the following exercises: Let the state at time $t_i$ be $z = z(t_i)$. Calculate the conditioned probabilities for

(i) $z(t_i)$ being a local maximum,

---

*This apparently non-objective character of entropy is often complained about. But this criticism is based on a misconception, since the term thermodynamical system is not defined without a choice for $\Omega_{\omega_0}$. This is no different in phenomenological thermodynamics, where the choice of ‘work degrees of freedom’, $\{y^i\}$, (the ‘relevant’ or ‘controlled’ degrees of freedom) is part of the definition of ‘system’. Only after they have been specified can one define the one-form of heat, called $\omega$, as the difference between the differential of total energy, $dE$, and the one-form of reversible work, called $\alpha := f_i dy^i$; hence $\omega := dE - \alpha$. Note that neither $\omega$ nor $\alpha$ are exact. In particular, $\omega \neq dQ$ for some function of state $Q$. In contrast to $E$, which is a function of states, $\omega$ and $\alpha$ are each a function of processes, which means that given a curve $\gamma$ on the manifold of (equilibrium) states, $\omega$ and $\alpha$ can be evaluated on (i.e. integrated along) $\gamma$. But it is meaningless to ask for the ‘value’ of heat and work on states. The value of heat associated to a process depends on the choice of $\alpha$, which in turn depends on the choice of ‘relevant’ $\{y^i\}$. Roughly speaking, heat is the amount of energy not transmitted in the channels (degrees of freedom) controlled by the $\{y^i\}$. This dependence of heat on the $\{y^i\}$ is directly inherited by entropy $S$, through $T dS = \omega$, where $T$ (temperature) and $S$ (entropy) are functions of state. They exist if and only if $\omega$ has an integrating factor (here $1/T$), which is the case if and only if $\omega \wedge dw = 0$, or in differential-geometric terminology, if the kernel distribution of $\omega$ is integrable. This integrability is, in turn, equivalent to the statement that in any neighbourhood of a given state there is another state that cannot be connected to the given one by a process (curve) on which the value of $\omega$ vanishes. To require that this latter be the case is just Carathéodory’s principle of adiabatic inaccessibility (Carathéodory, 1909), which allows to deduce the existence of $S$ and whose dependence on $\{y^i\}$ is now obvious.*
(ii) $z(t_i)$ being a local minimum,

(iii) $z(t_i)$ lying on a segment of positive slope,

(iv) $z(t_i)$ lying on a segment of negative slope.

Let the corresponding probabilities be $W_{\max}(z)$, $W_{\min}(z)$, $W_{\up}(z)$, and $W_{\down}(z)$, respectively. These are each given by the product of one past and one future conditioned probability. This being a result of the Markovian character of the dynamics, i.e. that for given $(z, t_i)$ the dynamical evolution $(z; t_i) \rightarrow (z \pm 1; t_{i+1})$ is independent of $z(t_{i-1})$. Using (28-29) we obtain:

$$W_{\max}(z) = W_{av}(z-1|z)W_{ret}(z-1|z) = \left(\frac{z}{N}\right)^2,$$

$$W_{\min}(z) = W_{av}(z+1|z)W_{ret}(z+1|z) = \left(1 - \frac{z}{N}\right)^2,$$

$$W_{\up}(z) = W_{av}(z-1|z)W_{ret}(z+1|z) = \frac{z}{N}\left(1 - \frac{z}{N}\right),$$

$$W_{\down}(z) = W_{av}(z+1|z)W_{ret}(z-1|z) = \frac{z}{N}\left(1 - \frac{z}{N}\right).$$

For $z/N > \frac{1}{2}$ ($z/N < \frac{1}{2}$) the probability $W_{\max}$ ($W_{\min}$) dominates the other ones. Expressed in terms of $\sigma$ the ratios of probabilities are given by the simple expressions:

$$W_{\max}(\sigma) : W_{\min}(\sigma) : W_{\up}(\sigma) : W_{\down}(\sigma) = \frac{1+\sigma}{1-\sigma} : \frac{1-\sigma}{1+\sigma} : 1 : 1. \quad (36)$$

In the limiting case of infinitely many $t_i$ we get that the state $z$ is $z^2/(N^2-z^2) = (1+\sigma)^2/2(1-\sigma)$ times more often a maximum than any other of the remaining three possibilities.

We also note an expression for the expected recurrence time, $T(z)$, for the state $z$. It is derived in Kac (1947) (there formula (66)). If the draws from the urns have constant time separation $\Delta t$ one has

$$T(z) = \frac{\Delta t}{W_{av}(z)},$$

and hence a connection between mean recurrence time and entropy:

$$S(z) = \ln \left[ \frac{2^N \Delta t}{T(z)} \right]. \quad (38)$$

Kac (1947) also shows the recurrence theorem, which for discrete state spaces asserts the recurrence of each state with certainty. More precisely: let $W'(z'; t_{i+n} | z; t_i)$ be the probability that for given state $z$ at time $t_i$ the state $z'$ occurs at time $t_{i+n}$ for the first time after $t_i$ (this distinguishes $W'$ from $W$), then $\sum_{n=1}^{\infty} W'(z; t_{i+n} | z; t_i) = 1$.

\footnote{Note that we talk about recurrence in the space $\Omega$ of macrostates ('coarse grained' states), not in the space $\Gamma$ of microstates.}
5.3 Coarse grained Gibbs entropy and the H-theorem

We recall that the Gibbs entropy $S_G$ lives on the space of probability distributions (i.e., normed measures) on $\Gamma$ and is hence independent of the choice of $\mathcal{O}_{re}$. In contrast, the coarse grained Gibbs entropy, $S_G^{cg}$, lives on the probability distributions on $\Omega$, $S_G^{cg} : \mathcal{W} \to \mathbb{R}$, and therefore depends on $\mathcal{O}_{re}$. Since the former does serve, after all, as a $\mathcal{O}_{re}$ independent definition of entropy (even though, thermodynamically speaking, not a very useful one), we distinguish the latter explicitly by the superscript ‘$cg$’. If at all, it is $S_G^{cg}$ and not $S_G$ that thermodynamically can be compared to $S_B$. The function $S_G^{cg}$ is given by

$$S_G^{cg}(W) = - \sum_{z=0}^N W(z) \cdot \ln \left[ \frac{W(z)}{W_{stat}(z)} \right]. \quad (39)$$

The structure of this expression is highlighted by means of the generalized H-theorem, which we explain below. Since the two entropies $S_B$ and $S_G^{cg}$ are defined on different spaces, $\Omega$ and $\mathcal{W}$, it is not immediately clear how to compare them. To do this, we would have to agree on what value of $S_G^{cg}$ we should compare with $S_B(z)$, i.e., what argument $W \in \mathcal{W}$ should correspond to $z \in \Omega$. A natural candidate is the distribution centered at $z$, that is, $W(z') = \delta(z')$, which is 1 for $z' = z$ and zero otherwise. From (39) we then obtain

$$S_G^{cg}(\delta_z) = S_B(z) - N \ln 2. \quad (40)$$

Let us now turn to the generalized H-theorem. Let $\Phi : \mathbb{R} \to \mathbb{R}$ be a convex function. Then for any finite family $m := \{x_1, \ldots, x_n\}$ of not necessarily pairwise distinct points in $\mathbb{R}$ we have the following inequality $\Phi(\sum_i a_i x_i) \leq \sum_i a_i \Phi(x_i) \forall a_i \in \mathbb{R}_{\geq 0}$ with $\sum_i a_i = 1$, where equality holds iff there is no index pair $i, j$, such that $x_i \neq x_j$ and $a_i \cdot a_j \neq 0$. In the latter case the convex sum is called trivial. We now define a function $H : \mathcal{W} \times \mathcal{W} \to \mathbb{R}$ through

$$H(W, W') := \sum_{z=0}^N W'(z) \Phi \left[ \frac{W(z)}{W'(z)} \right]. \quad (41)$$

Consider a time evolution $W_i \mapsto W_{i+1}$, $W_{i+1}(z) := \sum_z W(z|z')W_i(z')$, where clearly $W(z|z') \geq 0$ and $\sum_z W(z|z') = 1$. We also assume that no row of the matrix $W(z|z')$ just contains zeros (which would mean that the state labelled by the corresponding row number is impossible to reach). We call such time evolutions and the corresponding matrices non-degenerate. In what follows those distributions $W \in \mathcal{W}$ for which $W(z) > 0 \forall z$, i.e., from the interior of $\mathcal{W}$, will play a special role. We call them generic. The condition on $W(z|z')$ to be non-degenerate then ensures that the evolution leaves the set of generic distributions invariant. After these preparations we formulate

\footnote{Usually this expression is called the relative entropy $[W \text{ relative to } W_{\text{stat}}]$. As [absolute] entropy of $W$ one then understands the expression $- \sum_z W(z) \ln W(z)$. The H-theorem would be valid for the latter only if the constant distribution (in our case $W(z) = 1/(N+1)$) is an equilibrium distribution, which is not true for the urn model.}
**Theorem 8** (generalized H-theorem). Let \( W_i' \) be generic and the time evolution non-degenerate; then \( H(W_{i+1}, W_{i+1}') \leq H(W_i, W_i') \).

**Proof.** (Adaptation of the proof of theorem 3 in [Kubo (1981)] for the discrete case.) We define a new matrix \( V(z, z') := [W_{i+1}'(z)]^{-1}W(z|z')W_i'(z') \), which generates the time evolution for \( W_i(z)/W_i'(z) \) and obeys \( \sum_{z'} V(z|z') = 1 \). It follows:

\[
H(W_{i+1}, W_{i+1}') = \sum_{z=0}^{N} W_{i+1}'(z) \Phi \left[ \frac{W_{i+1}(z)}{W_{i+1}'(z)} \right] \tag{42}
\]

\[
= \sum_{z=0}^{N} W_{i+1}'(z) \Phi \left[ \sum_{z'=0}^{N} V(z|z') \frac{W_i(z')}{W_i'(z')} \right] \tag{43}
\]

\[
\leq \sum_{z'=0}^{N} \sum_{z=0}^{N} W_{i+1}'(z) V(z|z') \Phi \left[ \frac{W_i(z')}{W_i'(z')} \right] \tag{44}
\]

\[
= \sum_{z'=0}^{N} W_i'(z') \Phi \left[ \frac{W_i(z')}{W_i'(z')} \right] \tag{45}
\]

\[
= H(W_i, W_i'). \tag{46}
\]

Equality in (44) holds, iff the convex sum in the square brackets of (43) is trivial.

Picking a stationary distribution for \( W' \), which in our case is the unique distribution \( W_{stat} \), then \( H \) is a function of just one argument which does not increase in time. Taking in addition the special convex function \( \Phi(x) = x \ln(x) \), then we obtain with \( S^G \) := \(-H\) the above mentioned entropy formula.

Let from now on \( \Phi \) be as just mentioned. Then we have, due to \( \ln(x) \geq 1 - x^{-1} \), with equality iff \( x = 1 \):

\[
H(W, W') = \sum_{z=0}^{N} W(z) \ln \left[ \frac{W(z)}{W'(z)} \right] \geq \sum_{z=0}^{N} (W(z) - W'(z)) = 0, \tag{47}
\]

\[
\iff W(z) = W'(z) \forall z. \tag{48}
\]

Let us denote by a *distance function* on a set \( M \) any function \( d : M \times M \rightarrow \mathbb{R}_{\geq 0} \), such that \( d(x, y) = d(y, x) \) and \( d(x, y) = 0 \iff x = y \). (This is more general than a *metric*, which in addition must satisfy the triangle inequality.) A map \( \tau : M \rightarrow M \) is called non-expanding with respect to \( d \), iff \( d(\tau(x), \tau(y)) \leq d(x, y) \forall x, y \in M \). We have

**Theorem 9.** \( D : \hat{W} \times \hat{W} \rightarrow \mathbb{R}, D(W, W') := H(W, W') + H(W', W) \) is a distance function with respect to which every proper non-degenerate time evolution is non-expanding.

**Proof.** Symmetry is clear and (48) immediately implies \( D(W, W') \geq 0 \) with equality iff \( W = W' \), as follows from the separate positivity of each summand. Likewise (46) holds for each summand, so that no distance increases. 

\[
\blacksquare
\]
In this section we wish to show how to get a deterministic evolution for random variables in the limit $N \to \infty$. To this end we first consider the discrete, future directed time evolution of the expectation value of the random variable $X(z) = z$. We have

$$E(X_{t_{i+1}}) = \sum_{z' = 0}^N z' W_{i+1}(z') = \sum_{z' = 0}^N \sum_{z = 0}^N z' W_{ret}(z'|z) W_i(z)$$

$$= \sum_{z = 0}^N \left[(z+1)\frac{N-z}{N} + (z-1)\frac{z}{N}\right] W_i(z)$$

$$= 1 + \left(1 - \frac{2}{N}\right) E(X_{t_i}).$$

In the same way we get

$$E(X^2_{t_{i+1}}) = \sum_{z = 0}^N \left[(z+1)^2\frac{N-z}{N} + (z-1)\frac{z}{N}\right] W_i(z)$$

$$= 1 + 2E(X_{t_i}) + (1 - 4/N) E(X^2_{t_i}),$$

$$V(X_{t_{i+1}}) = E(X^2_{t_{i+1}}) - E^2(X_{t_{i+1}})$$

$$= (1 - 4/N) V(X_{t_i}) + \frac{4}{N} E(X_{t_i}) - \frac{4}{N^2} E^2(X_{t_i}).$$

By the evolution being ‘future directed’ one means that $W_{ret}$ and not $W_{av}$ are used in the evolution equations, as explicitly shown in (49). In this case one also speaks of ‘forward-directed evolution’.

In order to carry out the limit $N \to \infty$ we use the new random variable $\Sigma : \Omega \to \sigma$, where $\sigma = \frac{N}{2} - 1$ as above; hence $X = \frac{N}{2}(1 + \Sigma)$. Simple replacement yields

$$E(\Sigma_{t_{i+1}}) = (1 - 2/N) E(\Sigma_{t_i}),$$

$$V(\Sigma_{t_{i+1}}) = (1 - 4/N) V(\Sigma_{t_i}) + \frac{4}{N^2} \left(1 - E^2(\Sigma_{t_i})\right).$$

In order to have a sizable fraction of balls moved within a macroscopic time span $\tau$, we have to appropriately decrease the time steps $\Delta t := t_{i+1} - t_i$ with growing $N$, e.g. like $\Delta t = \frac{2}{N^2} \tau$, where $\tau$ is some positive real constant. Its meaning is to be the time span, in which $N/2$ balls change urns. Now we can take the limit $N \to \infty$ of (53) and (54),

$$\frac{d}{dt} E(\Sigma, t) = -\frac{1}{\tau} E(\Sigma, t) \implies E(\Sigma, t) = E_0 \exp\left(\frac{-(t - t_1)}{\tau}\right),$$

$$\frac{d}{dt} V(\Sigma, t) = -\frac{2}{\tau} V(\Sigma, t) \implies V(\Sigma, t) = V_0 \exp\left(\frac{-2(t - t_2)}{\tau}\right).$$
where $E_0, V_0, t_1, t_2$ are independent constants. These equations tell us, that 1) the expectation value approaches the equilibrium value $\Sigma = 0$ exponentially fast in the future, and 2) it does so with exponentially decaying standard deviation. The half mean time of both quantities is the time for $N/2$ draws.

According to the discussions in previous sections it is now clear, that in case of equilibrium identical formulae would have emerged if $W_{av}$ instead of $W_{ret}$ had been used, for then $W_{av} = W_{ret}$. Most importantly to note is, that the backward evolution is not obtained by taking the forward evolution and replacing in it $t \mapsto -t$. The origin of this difference is the fact already emphasized before (following Theorem 2), that $W_{av}(z; z')$ is not the inverse matrix to $W_{ret}(z; z')$, but rather the matrix computed according to Bayes’ rule.

7 Appendix

In this Appendix we collect some elementary notions of probability theory, adapted to our specific example.

The space of elementary events is $\Omega = \{0, 1, \ldots, N\}$. By

$$
\mathcal{X} := \{X : \Omega \rightarrow \mathbb{R}\},
$$

$$
\mathcal{W} := \{W : \Omega \rightarrow \mathbb{R}_{\geq 0} \mid \sum_{z \in \Omega} W(z) = 1\},
$$

we denote the sets of random variables and probability distributions respectively, where $\mathcal{W} \subset \mathcal{X}$. The map $\mathcal{X} \rightarrow \mathbb{R}^{N+1}$, $X \mapsto (X(0), X(1), \ldots, X(N))$ defines a bijection which allows us to identify $\mathcal{X}$ with $\mathbb{R}^{N+1}$. This identifies $\mathcal{W}$ with the $N$-simplex

$$
\Delta^N := \{(W(0), \ldots, W(N)) \in \mathbb{R}^{N+1} \mid 0 = W(i_1) = \cdots = W(i_K)\},
$$

Its boundary, $\partial \Delta^N$, is the union of all $(N - K)$-simplices:

$$
\Delta^{i_1 \cdots i_K} := \{(W(0), \ldots, W(N)) \in \Delta^N \mid 0 = W(i_1) = \cdots = W(i_K)\},
$$

for all $K$. Its interior is $\mathcal{W}^\circ := \mathcal{W} - \partial \mathcal{W}$, so that $W \in \mathcal{W}^\circ \iff W(z) \neq 0 \forall z$.

Expectation value $E$, variance $V$, and standard deviation $S$ are functions $\mathcal{X} \times \mathcal{W} \rightarrow \mathbb{R}$, defined as follows:

$$
E : \mathcal{X} \times \mathcal{W} \rightarrow \mathbb{R}, \quad E(X, W) := \sum_{z \in \Omega} X(z) W(z),
$$

$$
V : \mathcal{X} \times \mathcal{W} \rightarrow \mathbb{R}_{\geq 0}, \quad V(X, W) := E((X - \langle X \rangle)^2, W) = E(X^2, W) - E^2(X, W),
$$

$$
S : \mathcal{X} \times \mathcal{W} \rightarrow \mathbb{R}_{\geq 0}, \quad S(X, W) := \sqrt{V(X, W)},
$$

11‘Elementary’ is merely to be understood as mathematical standard terminology, not in any physical sense. For example, in the urn model, $\Omega$ is obtained after coarse graining from the space of physically ‘elementary’ events.
where in (62) $\langle X \rangle$ simply denotes the constant function $\langle X \rangle : z \mapsto E(X, W)$, and $E^2(X, W) := [E(X, W)]^2$. In the main text we also write $E(X, s)$ if the symbol $s$ uniquely labels a point in $W$, like $s = ap$ for the a priori distribution $[1]$, or $E(X, t_i)$ for the distribution $W_i$ at time $t_i$.

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