ON THE STATISTICAL VIEWPOINT CONCERNING THE 2nd LAW OF THERMODYNAMICS

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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 try to explain this statement—which is well known since the time of the Ehrenfests—in some detail within a systematic Bayesian approach.

1 Introduction

First, we wish to make the statement in the abstract more precise. To this end, we think of an idealized 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. A 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 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 from 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 1. 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 also a likely increase.

Consequence 2. 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 3. 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 finite time-interval and imposing a low-entropy condition at one of the two *ends* of the interval. Without further structural elements which would allow to distinguish the two ends, the apparently existing *two* possibilities to do so 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 end, where the condition is placed.

Many notions any types of reasoning in statistical thermodynamics can be well illustrated in terms of the Ehrenfest's urn-model, which is to be regarded as a toy model of a thermodynamic system, and whose detailed description we present below. In particular, this holds true for the consequences listed above, for whose partial illustration this model was designed by Paul and Tatiana Ehrenfest [1]; see also [2]-[5]. Our presentation will be more detailed than theirs. Nothing of what we say will be essentially new. Besides being more detailed, we try to take a Bayesian approach. In what follows it will be important to alway relate to the general formalism of statistical thermodynamics in order to not provoke 'easy' or 'intuitive' but uncontrolled reasonings. There is always a certain danger for this to happen in the context of simple models. The Appendix collects some elementary notions which are not explained in the main text. These will be relevant in the following section.

2 The Urn-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 numbers of balls contained in U_1 (the complementary set of numbers then label the balls in U_0). To formalize 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 Γ (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 Γ carries a natural measure, μ_Γ, given by associating to each subset $\Lambda \subset \Gamma$ its cardinality: $\mu_\Gamma(\Lambda) = |\Lambda|$. We now make the physical assumption, that the probability measure (normalized measure) $\nu_\Gamma := 2^{-N}\mu_\Gamma$ 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 $\emptyset$. Conversely, it is generally impossible to associate a physically realizable observable to any element in $\emptyset$. Let $\{O_1, \ldots, O_n\} =: \emptyset_{re} \subset \emptyset$ the physically realizable ones [1], which we can combine into a single n component observable $O_{re} \in \emptyset^n$. 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 in 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 Γ: $\Gamma_\alpha \cap \Gamma_\beta = \emptyset$ if $\alpha \neq \beta$ and $\bigcup_{\alpha\in\Omega} \Gamma_\alpha = \Gamma$.

The realized 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 Γ_z of $\binom{N}{z}$ microstates. The probability measure ν_Γ induces so-called a priori probabilities for macrostates z:

$$W_{ap}(z) = \nu_\Gamma(\Gamma_z) = 2^{-N}\binom{N}{z}. \tag{1}$$

Let$X : \Omega \to \mathbb{R}$ be the random variable $z \mapsto X(z) = z$. Its expectation value E and

[1] The subscript 're' can be read as abbreviation for 'realized' or 'relevant'.

standard deviation S with respect to the a priori distribution (1) are given by[2]

$$E(X, \mathrm{ap}) = \frac{N}{2}, \tag{2}$$

$$S(X, \mathrm{ap}) = \frac{\sqrt{N}}{2}. \tag{3}$$

The system has a Markoffian random evolution, which is defined as follows: at every discrete lying time t_i, where $i = \{0, 1, 2, \cdots\}$ 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 $z \to z + 1$. Alternatively, the ball has been in U_1 and the change of macrostate is given by $z \to z - 1$. 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

$$W(z+1; t_{i+1}|z; t_i) = \frac{N-z}{N} =: W_{\mathrm{ret}}(z+1|z), \tag{4}$$

$$W(z-1; t_{i+1}|z; t_i) = \frac{z}{N} =: W_{\mathrm{ret}}(z-1|z). \tag{5}$$

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* than z, that is, the probabilities are *past-conditioned* or *retarded*. We indicate this by writing W_{ret}.

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

$$\begin{aligned} W(z; t_{i+1}) &= W(z; t_{i+1}|z+1; t_i)\, W(z+1; t_i) \\ &+ W(z; t_{i+1}|z-1; t_i)\, W(z-1; t_i) \qquad (6) \\ &= \frac{z+1}{N} W(z+1; t_i) + \frac{N-z+1}{N} W(z-1; t_i), \qquad (7) \end{aligned}$$

[2]Note

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

$$E(X^2 - X; \mathrm{ap}) = 2^{-N} \sum_{z=2}^{N} z(z-1) \binom{N}{z} = 2^{-N} N(N-1) \sum_{m=0}^{N-2} \binom{N-2}{m} = \frac{N(N-1)}{4} \quad .$$

whose Markoffian 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_{stat} for $i \gg N$, where W_{stat} is independent of W_0. Its uniqueness is shown by

Theorem 1. *A distribution W_{stat} which is stationary under (7) is uniquely given by W_{ap} in (1).*

Proof. We show, that W_{stat} can be uniquely determined from (7). To this end, we assume a time independent distribution W_{stat} and write (7) in the form

$$W_{\text{stat}}(z+1) = \frac{N}{z+1} W_{\text{stat}}(z) - \frac{N-z+1}{z+1} W_{\text{stat}}(z-1). \tag{8}$$

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

$$\begin{aligned} W_{\text{stat}}(z+1) &= \left[\frac{N}{z+1}\binom{N}{z} - \frac{N-z+1}{z+1}\binom{N}{z-1}\right] W_{\text{stat}}(0) \\ &= (N-z)\frac{N(N-1)\cdots(N-z+1)}{(z+1)!} W_{\text{stat}}(0) \\ &= \binom{N}{z+1} W_{\text{stat}}(0). \end{aligned} \tag{9}$$

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

$$1 = \sum_{z=0}^{n} W_{\text{stat}}(z) = W_{\text{stat}}(0) \sum_{z=0}^{N} \binom{N}{z} = W_{\text{stat}}(0)\, 2^N \Rightarrow W_{\text{stat}}(0) = 2^{-N}. \tag{10}$$

□

2.1 Future-conditioned probabilities and Bayes' rule

Given a probability space and a set of events, $\{A_1, \ldots, A_n\}$, which is 1.) complete, i.e. $A_1 \cup \cdots \cup A_n = \mathbf{1}$ (here $\mathbf{1}$ denotes the certain event), and 2.) mutually exclusive, i.e. $i \neq j \Rightarrow A_i \cap A_j = \mathbf{0}$ (here $\mathbf{0}$ denotes the impossible event). The probability of an event B then obeys *Bayes' rule*[3]: $W(B) = \sum_{k=1}^{n} W(B|A_k)W(A_k)$. This is just

[3] We deliberately avoid to call it Bayes' theorem.

what we used in (6). This rule now allows us to deduce the inversely conditioned probabilities:

$$W(A_k|B) = \frac{W(B|A_k)W(A_k)}{\sum_{i=1}^{n} W(B|A_i)W(A_i)}. \tag{11}$$

We now identify the A_i with the $N+1$ events $(z'; t_i)$ at the fixed time t_i, where $z' = 0, \ldots, N+1$, and A_k with the special event $(z \pm 1; t_i)$. Further we identify the event B with $(z; t_{i+1})$, i.e. with the occurrence of z at the *later* time t_{i+1}. Then we obtain:

$$\begin{aligned} W(z \pm 1; t_i \mid z; t_{i+1}) &= \frac{W(z; t_{i+1}|z \pm 1; t_i)W(z \pm 1; t_i)}{\sum_{z'=0}^{N} W(z; t_{i+1}|z'; t_i)W(z'; t_i)} && (12) \\ &= \frac{W(z; t_{i+1}|z \pm 1; t_i)W(z \pm 1; t_i)}{W(z; t_{i+1})}. && (13) \end{aligned}$$

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 (4-5). 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:

$$\begin{aligned} W(z+1; t_i|z; t_{i+1}) &= \frac{W(z+1; t_i)}{W(z+1; t_i) + \frac{N-z+1}{z+1} W(z-1; t_i)}, && (14) \\ W(z-1; t_i|z; t_{i+1}) &= \frac{W(z-1; t_i)}{W(z-1; t_i) + \frac{z+1}{N-z+1} W(z+1; t_i)}. && (15) \end{aligned}$$

2.2 Flow equilibrium

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

$$W(z \pm 1; t_{i+1}|z; t_i)W(z; t_i) = W(z; t_{i+1}|z \pm 1; t_i)W(z \pm 1; t_i). \tag{16}$$

It already implies $W_i = W_{ap}$, since (4-5) give[4] $W(z+1; t_i) = \frac{N-z}{z+1} W(z; t_i)$ which leads to $W(z; t_i) = \binom{N}{z} W(0; t_i)$. Since $1 = \sum_z W(z; t_i)$ we have $W(0; t_i) =$

[4] Without using (4-5) one gets

$$\begin{aligned} W(z \pm 1; t_{i+1}|z; t_i)W(z; t_i) &= W(z; t_{i+1}|z \pm 1; t_i)W(z \pm 1; t_i) \\ &= W(z \pm 1; t_i|z; t_{i+1})W(z; t_{i+1}) && (17) \end{aligned}$$

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 (cf. 19)

$$\frac{W(z \pm 1; t_{i+1}|z; t_i)}{W(z \pm 1; t_i|z; t_{i+1})} = \frac{W(z; t_{i+1})}{W(z; t_i)}. \tag{18}$$

2^{-N}. Using Theorem 1, we conclude that flow equilibrium at t_i implies $W_j = W_{ap}$ for $j \geq i$.

2.3 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:

$$\begin{aligned} W(z \pm 1; t_{i+1}|z; t_i) &= W(z \pm 1; t_i|z; t_{i+1}) && (19)\\ &\overset{(13)}{=} W(z; t_{i+1}|z \pm 1; t_i)\frac{W(z \pm 1; t_i)}{W(z; t_{i+1})}, && (20)\\ \overset{(4,5)}{\Longleftrightarrow} \quad W(z; t_{i+1}) &= \frac{z+1}{N-z} W(z+1; t_i) && (21)\\ &= \frac{N-z+1}{z} W(z-1; t_i). && (22) \end{aligned}$$

It is interesting to note that the condition of time-reversal invariance is weaker that that of flow equilibrium. The former is implied, but does not itself imply the equilibrium distribution. Let us explain this in more detail: Equations (21-22) imply (7), since $\frac{N-z}{N} \times (21) + \frac{z}{N} \times (22) = (7)$. Hence (21-22) are stable under time evolution (7). Conversely, (21-22) is implied by (7) and the following equation, expressing the equality of the right hand sides of (21) and (22):

$$W(z+1; t_i) = \frac{N-z}{z+1}\frac{N-z+1}{z} W(z-1; t_i). \tag{23}$$

Indeed, eliminating $W(z+1; t_i)$ in (7) using (23), one gets

$$W(z; t_{i+1}) = \frac{N-z+1}{z} W(z-1; t_i) \overset{(18)}{=} \frac{z+1}{N-z} W(z+1; t_i), \tag{24}$$

hence (21-22). Time-reversal invariance for future times is therefore equivalent to the 'constraint' (23) 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 $W_i(z) = p\binom{N}{z}$ for z even and $W_i(z) = \frac{q}{N}\binom{N}{z}$ 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 $1 = 2^{N-1}(p + \frac{q}{N}) \Rightarrow q = N(2^{-(N-1)} - p)$. This shows that $p \in [0, 2^{-(N-1)}]$ faithfully parameterizes all distributions obeying (23). One should note that solutions to (23) 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, $W^e(z) = (1-(-1)^{z-1})2^{-N}\binom{N}{z}$ and 'odd'

distribution, $W^o(z) = (1-(-1)^z)2^{-N}\binom{N}{z}$. Solutions to (23) form a closed interval within the simplex Δ^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 $\Delta^{24\cdots N}$. If we call this interval Δ^*, we have

Theorem 2. *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 $W(z;t_i|z';t_{i+1})$ coincide.*[5]

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.

3 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:

$$W_{ret}(z+1|z) = W_{av}(z+1|z) = \frac{N-z}{N}, \tag{27}$$

$$W_{ret}(z-1|z) = W_{av}(z-1|z) = \frac{z}{N}, \tag{28}$$

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 $\frac{z}{N}$. 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] Explicitly one can see the preservation of (23) under time evolution (7) as follows: Given that the initial distribution W_i satisfies (23), the development (7) is equivalent to (21-22). Hence

$$W(z-1;t_i) = \frac{z}{N-z+1}\,W(z;t_{i+1}) \tag{25}$$

$$W(z+1;t_i) = \frac{z+2}{N-z-1}\,W(z+2;t_{i+1}) \tag{26}$$

which allows to rewrite (23) for W_i into (23) for W_{i+1}.

3.1 Boltzmann Entropy

Boltzmann Entropy S_B is a function $S_B : \Omega \to \mathbb{R}$. We stress that since Ω is defined only *after* a choice of coarse graining (i.e. a choice of $\emptyset_{re}$) has been made, Boltzmann Entropy, too, must be understood as relative to that choice.[6] The value $S_B(z)$ in the macro state z is defined by $S_B(z) := \ln \mu_\Gamma(\Gamma_z)$. 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:

$$S_B(z) = N \ln N - z \ln z - (N - z) \ln(N - z), \tag{29}$$

$$S_B(\sigma) = -\frac{N}{2}\left[\ln \frac{1-\sigma^2}{4} + \sigma \ln \frac{1+\sigma}{1-\sigma}\right]. \tag{30}$$

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 $|\sigma|$, $S_B : [0, 1] \to [\ln 2^N, 0]$ is strictly monotonically decreasing. That $S_B(\sigma = 1) = 0$ is best seen in the limit $z \to N$ of (29). 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.

3.2 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 $z(t_i)$ i) a local maximum, ii) a local minimum, iii)

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

[6] 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 $\emptyset_{re}$. 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 differential one-form of heat, δQ, as the difference between the differential of total energy, dE, and the differential one-form of reversible work, $\delta A := f_i dy^i$. (Here δ is just meant to indicate that the quantity in question is a one-form, not that it is the differential, d, of a function; i.e. $d\delta A \neq 0$ and $d\delta Q \neq 0$ in general.) Hence we *define* $\delta Q := dE - \delta A$. Roughly speaking, one may say that 'heat' is the energy that is localized in the non-relevant (not controlled) degrees of freedom.

(ii) $z(t_i)$ being a local minimum,

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

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

Let the corresponding probabilities be $W_{\max}(z)$, $W_{\min}(z)$, $W_{\uparrow}(z)$, and $W_{\downarrow}(z)$ respectively. These are each given by the product of one past and one future conditioned probability. This being a result of the Markoffian character of the dynamics, i.e. that for given (z, t_i) the dynamical evolution $(z; t_i) \to (z \pm 1; t_{i+1})$ is independent of $z(t_{i-1})$. Using (27-28) we obtain:

$$W_{\max}(z) = W_{\text{av}}(z-1|z)W_{\text{ret}}(z-1|z) = \left(\frac{z}{N}\right)^2, \tag{31}$$

$$W_{\min}(z) = W_{\text{av}}(z+1|z)W_{\text{ret}}(z+1|z) = \left(1-\frac{z}{N}\right)^2, \tag{32}$$

$$W_{\uparrow}(z) = W_{\text{av}}(z-1|z)W_{\text{ret}}(z+1|z) = \frac{z}{N}\left(1-\frac{z}{N}\right), \tag{33}$$

$$W_{\downarrow}(z) = W_{\text{av}}(z+1|z)W_{\text{ret}}(z-1|z) = \frac{z}{N}\left(1-\frac{z}{N}\right). \tag{34}$$

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 σ the ratios of probabilities are given by the simple expressions:

$$W_{\max}(\sigma) : W_{\min}(\sigma) : W_{\uparrow}(\sigma) : W_{\downarrow}(\sigma) = \frac{1+\sigma}{1-\sigma} : \frac{1-\sigma}{1+\sigma} : 1 : 1. \tag{35}$$

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.[7] It is derived in [5] (there formula (66)). If the draws from the urns have constant time separation Δt one has

$$T(z) = \frac{\Delta t}{W_{\text{ap}}(z)}, \tag{36}$$

and hence a connection between mean recurrence time and entropy:

$$S(z) = \ln\left[\frac{2^N \Delta t}{T(z)}\right]. \tag{37}$$

[7] Note that we talk about recurrence in the space Ω of macrostates ('coarse grained' states), not in the space Γ of microstates.

Reference [5] 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 $\sum_{n=1}^{\infty} W'(z; t_{i+n}|z; t_i) = 1$.

3.3 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 Γ and is hence independent of the choice of $\emptyset_{\text{re}}$. In contrast, the coarse grained Gibbs entropy, S_G^{cg}, lives on the probability distributions on Ω, $S_G^{cg} : \mathcal{W} \to \mathbb{R}$, and therefore depends on $\emptyset_{\text{re}}$. Since the former does serve, after all, as a $\emptyset_{\text{re}}$ 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 we be compared to S_B. The function S_G^{cg} is given by

$$S_G^{cg}(W) = -\sum_{z=0}^{N} W(z) \cdot \ln\left[\frac{W(z)}{W_{\text{stat}}(z)}\right]. \tag{38}$$

The structure of this expression is highlighted by means of the generalized H-theorem, which we explain below.[8] Since the two entropies S_B and S_G^{cg} are defined on different spaces, Ω 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, $W(z') = \delta_z(z')$, which is 1 for $z' = z$ and zero otherwise. From (38) we then obtain

$$S_G^{cg}(\delta_z) = S_B(z) - N \ln 2\,. \tag{39}$$

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 $\Phi(\sum_i \alpha_i x_i) \leq \sum_i \alpha_i \Phi(x_i)\, \forall\, \alpha_i \in \mathbb{R}_{\geq 0}$ with $\sum_i \alpha_i = 1$, where equality holds iff there is no index pair i, j, such that $x_i \neq x_j$ and $\alpha_i \cdot \alpha_j \neq 0$. In the latter case the convex sum

[8] Usually this expression is called the *relative* entropy [of W relative to W_{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.

is called trivial. We now define a function $H : \mathcal{W} \times \mathcal{W} \to \mathbb{R}$ through

$$H(W, W') := \sum_{z=0}^{N} W'(z)\Phi\left[\frac{W(z)}{W'(z)}\right]. \tag{40}$$

Consider a time evolution $W_i \mapsto W_{i+1}$, $W_{i+1}(z) := \sum_i W(z|z')W_i(z')$, 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 $\overset{\circ}{\mathcal{W}} \subset \mathcal{W}$, 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

Theorem 3 (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 [6] 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:

$$\begin{aligned}
H(W_{i+1}, W'_{i+1}) &= \sum_{z=0}^{N} W'_{i+1}(z)\,\Phi\left[\frac{W_{i+1}(z)}{\mathcal{W}'_{i+1}(z)}\right] && (41)\\
&= \sum_{z=1}^{N} W'_{i+1}(z)\,\Phi\left[\sum_{z'=0}^{N} V(z|z')\frac{W_i(z')}{W'_i(z')}\right] && (42)\\
&\leq \sum_{z'=0}^{N}\sum_{z=0}^{N} W'_{i+1}(z)V(z|z')\,\Phi\left[\frac{W_i(z')}{W'_i(z')}\right] && (43)\\
&= \sum_{z'=0}^{N} W'_i(z')\,\Phi\left[\frac{W_i(z')}{W'_i(z')}\right] && (44)\\
&= H(W_i, W'_i) && (45)
\end{aligned}$$

Equality in (43) holds, iff the convex sum in the square brackets of (42) 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 $S_G^{cg} := -H$ the above mentioned entropy formula.

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

$$\begin{aligned} H(W,W') &= \sum_{z=0}^{N} W(z)\,\ln\left[\frac{W(z)}{W'(z)}\right] \geq \sum_{z=0}^{N}(W(z)-W'(z)) = 0, \quad (46)\\ &= 0 \Longleftrightarrow W(z) = W'(z) \quad \forall z. \quad (47)\end{aligned}$$

Let us denote by a *distance function* on a set M any function $d : M \times M \to \mathbb{R}_{\geq 0}$, such that $d(x,y) = d(y,x)$ and $d(x,y) = 0 \Leftrightarrow x = y$. (This is more general than a *metric*, which in addition must satisfy the triangle inequality.) A map $\tau : M \to M$ 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 4. $D : \overset{\circ}{\mathcal{W}} \times \overset{\circ}{\mathcal{W}} \to \mathbb{R}$, $D(W,W') := H(W,W') + H(W',W)$ *is a distance function with respect to which every proper non-degenerate time evolution is non-expanding.*

Proof. Symmetry is clear and (47) immediately implies $D(W,W') \geq 0$ with equality iff $W = W'$, as follows from the separate positivity of each summand. Likewise (45) holds for each summand, so that no distance increases. □

4 Thermodynamic limit and deterministic dynamics

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

$$\begin{aligned} E(X,t_{i+1}) &= \sum_{z'=0}^{N} z' W_{i+1}(z') = \sum_{z'=0}^{N}\sum_{z=0}^{N} z' W_{\text{ret}}(z'|z) W_i(z) \quad (48)\\ &= \sum_{z=0}^{N}\left[(z+1)\frac{N-z}{N} + (z-1)\frac{z}{N}\right] W_i(z)\\ &= 1 + \left(1-\frac{2}{N}\right) E(X,t_i). \quad (49)\end{aligned}$$

In the same way we get

$$\begin{aligned} E(X^2, t_{i+1}) &= \sum_{z=0}^{N} \left[(z+1)^2 \frac{N-z}{N} + (z-1)\frac{z}{N} \right] W_i(z) \\ &= 1 + 2E(X, t_i) + (1 - 4/N)\, E(X^2, t_i) \end{aligned} \tag{50}$$

$$\begin{aligned} V(X, t_{i+1}) &= E(X^2, t_{i+1}) - E^2(X, t_{i+1}) \\ &= (1 - 4/N)\, V(X, t_i) + \frac{4}{N} E(X, t_i) - \frac{4}{N^2} E^2(X, t_i) \end{aligned} \tag{51}$$

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 (48). 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 $\sigma = \frac{2z}{N} - 1$ as above; hence $X = \frac{N}{2}(1 + \Sigma)$. Simple replacement yields

$$E(\Sigma, t_{i+1}) = (1 - 2/N)\, E(\Sigma, t_i) \tag{52}$$

$$V(\Sigma, t_{i+1}) = (1 - 4/N)\, V(\Sigma, t_i) + \frac{4}{N^2} \left(1 - E^2(\Sigma, t_i) \right). \tag{53}$$

In order to have a seizable fraction of balls moved within a macroscopic time span τ, we have to appropriately decrease the time steps $\Delta t := t_{i+1} - t_i$ with growing N, e.g. like $\Delta t = \frac{2}{N}\tau$, where τ 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 (52) and (53),

$$\frac{d}{dt} E(\Sigma, t) = -\frac{1}{\tau} E(\Sigma, t) \implies E(\Sigma, t) = E_0 \exp\left(\frac{-(t - t_1)}{\tau} \right), \tag{54}$$

$$\frac{d}{dt} V(\Sigma, t) = -\frac{2}{\tau} V(\Sigma, t) \implies V(\Sigma, t) = V_0 \exp\left(\frac{-2(t - t_2)}{\tau} \right), \tag{55}$$

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 $W_{\text{av}} = W_{\text{ret}}$. 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 $W_{\rm av}(z;z')$ is not the inverse matrix to $W_{\rm ret}(z;z')$, but rather the matrix computed according to Bayes' rule.

5 Appendix

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

The space of elementary events[9] is $\Omega = \{0, 1, \ldots, N\}$. By

$$\mathcal{X} : = \big\{X : \Omega \to \mathbb{R}\big\} \tag{56}$$

$$\mathcal{W} : = \big\{W : \Omega \to \mathbb{R}_{\geq 0} \mid \sum_{z\in\Omega} W(z) = 1\big\} \tag{57}$$

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

$$\Delta^N := \big\{(W(0), \cdots, W(N)) \in \mathbb{R}^{N+1} \mid W(z) \geq 0, \sum_z W(z) = 1\big\} \subset \mathbb{R}^{N+1}. \tag{58}$$

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

$$\Delta^{i_1\cdots i_K} := \big\{(W(0), \ldots, W(N)) \in \Delta^N \mid 0 = W(i_1) = \cdots = W(i_K)\big\} \tag{59}$$

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

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

$$E : \mathcal{X} \times \mathcal{W} \to \mathbb{R}, \qquad E(X, W) := \sum_{z\in\Omega} X(z)W(z) \tag{60}$$

$$V : \mathcal{X} \times \mathcal{W} \to \mathbb{R}_{\geq 0}, \quad V(X, W) := E((X - \langle X\rangle)^2, W) = E(X^2, W) - E^2(X, W) \tag{61}$$

$$S : \mathcal{X} \times \mathcal{W} \to \mathbb{R}_{\geq 0}, \quad S(X, W) := \sqrt{V(X, W)} \tag{62}$$

where in (61) $\langle X\rangle$ 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 $\mathcal{W}$, like $s = ap$ for the a priori distribution (1), or $E(X, t_i)$ for the distribution W_i at time t_i.

[9] 'Elementary' is merely to be understood as mathematical standard terminology, not in any physical sense. For example, in the urn model, Ω is obtained after coarse graining form the space of physically 'elementary' events.

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