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ENTROPY AND THE EHRENFEST URN MODEL

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Synopsis

This note concerns the entropy of the Ehrenfest urn model. Both Boltzmann and Gibbs entropies are discussed. It is shown that they agree at equilibrium. The Boltzmann entropy shows fluctuations in time while the Gibbs entropy is proved to increase monotonically to its maximum (equilibrium) value. The concepts of equilibrium associated with the two points of view are compared.

I. *Introduction.* In 1907 Paul and Tatiana Ehrenfest [1]) introduced a simple probability model designed to illustrate and to clarify Boltzmann's proof of the H-theorem. This urn model has attracted considerable attention [2])–[7]) both for its heuristic value in statistical mechanics and for its mathematical interest as a simple Markoff process.

This note deals with the entropy of the urn model considered as a physical system. Previous discussions have only drawn an analogy between the time variation of a quantity peculiar to the Ehrenfest model and the time variation of the entropy of a closed system. It is possible, however, to treat the entropy of the urn model itself and this treatment is carried out below.

The principal result of the analysis is to sharpen the distinction between the Boltzmann and the Gibbs definitions of the entropy. These definitions essentially coincide for a system in equilibrium because of what Lorentz [8]) calls "la remarquable insensibilité de la formule de Boltzmann". The time dependence of the two entropies is quite different: the Boltzmann entropy, based on the actual state of the system shows the kind of fluctuations familiar in discussions of the H-theorem, whereas the Gibbs entropy shows a monotonic increase with time, approaching a maximum value in the equilibrium state.

Although these distinctions are not new, and were actually first analyzed in detail by the Ehrenfests in their Enzyklopädie article [9]) [10]), the analysis has not previously been carried out for the simple system of the Ehrenfest urn model.

II. *The urn model and its entropy.* The model may be described in the following way. Consider two urns, A and B, and $2R$ balls, numbered consecu-

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tively from 1 to $2R$, which are distributed in these two urns. An integer between 1 and $2R$ is chosen at random in such a way that all these integers have equal probabilities of being chosen, and the ball with that number is moved from the urn in which it is located to the other urn. This procedure is repeated regularly at intervals of time τ.

The "macroscopic" state of the system is characterized, at any time, by the integer l where $R + l$ is the number of balls then in urn A (and $R - l$ is the number of balls in urn B). It is evident that l takes on values from the set $-R, -R + 1, \ldots, 0, \ldots, R - 1, R$. In contrast, the "microscopic" state of the system is given by enumerating the numbers of the $R + l$ balls in urn A. The word "state" without further designation will be used to mean macroscopic state.

The basic "equation of motion" of the urn model is a stochastic equation since a given initial state determines only the probabilities of the various states at a later time $s\tau$ (after s repetitions of the process). Let us define $P(n|m; s)$ as the probability that after s repetitions there are $R + m$ balls in urn A, given that there were $R + n$ balls in urn A initially. The stochastic equation is readily seen to be

$$P(n|m; s) = \frac{R+m+1}{2R} P(n|m+1; s-1) + \frac{R-m+1}{2R} P(n|m-1; s-1). \quad (1)$$

This equation expresses the probabilities at time $s\tau$ in terms of the probabilities at time $(s - 1)\,\tau$.

The solution of Eq. (1) subject to the initial condition $P(n|m; 0) = \delta_{nm}$ has been obtained by K a c [3]). Kac has shown (among other things) that for any initial state of the system the distribution eventually approaches the stationary or equilibrium distribution given by

$$P_0(m) = \alpha \frac{(2R)!}{(R+m)!\,(R-m)!} \equiv \alpha\, G_m. \quad (2)$$

Here $P_0(m)$ is the equilibrium probability that urn A contains $R + m$ balls and α is a normalization constant equal to 2^{-2R}. We note that $P_0(m)$ is proportional to G_m ($\equiv (2R)!/(R + m)!\,(R - m)!$) where G_m is the number of microscopic states all of which correspond to the macroscopic state m. This equilibrium distribution is stationary in the sense that it is unchanged by the stochastic equation, since it is easily verified that

$$P_0(m) = \frac{R+m+1}{2R} P_0(m+1) + \frac{R-m+1}{2R} P_0(m-1). \quad (3)$$

To summarize, we can say that the Ehrenfest model approaches equilibrium, where equilibrium is characterized by the probability distribution $P_0(m)$ for the various states m. This implies, of course, that the state m shows fluctuations even at equilibrium which can be calculated from the equilibrium distribution. The mean value and also the most probable value of m at equilibrium is zero, corresponding to equal distribution of the balls between urns A and B.

With this background we can now formulate the definitions of the entropy for the Ehrenfest system. Consider first the entropy according to Boltzmann's relation: the entropy is proportional to the logarithm of the number of microscopic states compatible with the given macroscopic state. From the discussion above we can then write for S, the Boltzmann entropy of the system in state m,

$$\mathsf{S} = \ln G_m = \ln ((2R)!/(R+m)!\,(R-m)!) \tag{4}$$

where S is expressed in units of Boltzmann's constant k. Using Stirling's approximation for the factorials S can be written as

$$\mathsf{S} = -\,(R+m)\ln(R+m) - (R-m)\ln(R-m) + \text{constant.} \tag{5}$$

We notice that the entropy defined by Eq. (4) depends on the actual state of the system, i.e. on the single parameter m. In previous discussions of the Ehrenfest model the time variation of m was taken as indicative of the time variation of the entropy, and we see that this point of view is appropriate when S is the entropy.

Let us now define the entropy from the Gibbsian standpoint. Here we take account of the stochastic nature of the system from the outset, and therefore we define an entropy S in terms of the probabilities for finding the system in states m. If we abbreviate the symbol $P(n|m;s)$ defined above as P_m then S is defined as

$$S = -\,\Sigma_{m=-R}^{R} P_m \ln (P_m/G_m) = -\,\Sigma_m P_m \ln P_m + \Sigma_m P_m \ln G_m. \tag{6}$$

In the usual Gibbsian terminology of ensembles P_m can be expressed as follows. Imagine many replicas of the Ehrenfest urns each of which initially has $R+n$ balls in its A urn. Then P_m is the fraction of the total number of urn models which at time $s\tau$ have $R+m$ balls in their A urns.

The second form of Eq. (6) shows us the general relationship between S and S. We see that S is the average of S, $(\Sigma_m P_m \ln G_m)$, plus a term $(-\,\Sigma_m P_m \ln P_m)$ which measures the extent to which the various states are occupied.

III. *The entropy at equilibrium.* Let us now compare the two entropy definitions for the equilibrium state of the system. We must first point out, however, that the two concepts of equilibrium state are different. From the Boltzmann point of view the equilibrium state is indeed a state, i.e. a macroscopic state, of the urn model. It is that state for which the entropy S is a maximum. The equilibrium state is then the state $m = 0$, corresponding to equal numbers of balls in the two urns. Since this state means, in probability language, $P_m = \delta_{m0}$, a distribution which is not a stationary solution of the basic stochastic equation, Eq. (1), it follows that there will be departures from the equilibrium state, i.e. fluctuations *about* equilibrium.

From the Gibbs standpoint equilibrium is characterized by a probability distribution rather than by a particular state. It is that distribution for which S is a maximum, and this is readily seen to be the distribution $P_m = P_0(m) = \alpha\, G_m$. This distribution *is* stationary in time so that once it is reached it persists. Since, however, equilibrium corresponds to a probability distribution rather than a state, we now have fluctuations *at* equilibrium, fluctuations which are, so to speak, a part of our concept of equilibrium.

Now let us write down the values of the two entropies, S and S, at equilibrium to show that, despite the rather considerable difference in meaning, the values of S_{eq} and S_{eq} are essentially the same.

For S we have the expression

$$\mathsf{S}_{eq} = \ln G_0 = \ln (2R)!/R!R! = 2R \ln 2. \tag{7}$$

For S we can write the expression

$$S_{eq} = -(\ln \alpha)\, \Sigma_m\, P_0(m) = 2R \ln 2. \tag{8}$$

Hence, if R is large enough to justify the use of Stirling's formula, the two entropies have precisely the same value at equilibrium. It is only for the non-equilibrium case that the difference in viewpoint is reflected in a difference in the behaviour of S and S, and to this case we now turn our attention.

IV. *Time dependence of the entropy.* We begin by considering the entropy S which is a function of the actual state of the system (i.e. the number of balls in urn A) as this state changes with time. Since the variation of the state m with time is determined by the stochastic equation, Eq. (1), S is a stochastic function, a function of the stochastic variable m. We may point out that it follows from Eq. (5) that S actually depends only on $|m|$, which is clear from the symmetry of the problem with respect to urns A and B. The kind of variation shown by S is made evident by the experimental results of Schrödinger and Kohlrausch who actually carried out the Ehrenfest lottery. Their results have recently been replotted by Ter Haar [11]). We have not made any new calculations here because previous results suffice to establish the important points.

First, since, as Kac has proved, every state is bound to recur with probability one, arbitrarily small values of the entropy S are certain to be found. Second, since the recurrence time of any state m is proportional to τ/G_m it follows that values of S differing from S_{eq} occur more rarely as the difference between S_{eq} and S increases.

Roughly speaking, then, S will tend to approach S_{eq}, showing fluctuations in the approach and will then continue to fluctuate indefinitely. We may mention that $\langle S \rangle$, the average value of S, i.e. the sum of the values of S in the possible states times the respective probabilities of occurrence of these states, does not show a monotonically increasing behaviour in time. This can easily be seen if one starts from the state $m = 0$.

Consider now the time dependence of S. We shall prove that S increases monotonically with time, i.e. that $S(s + 1) \geq S(s)$. Before writing this out explicitly we change variables for convenience. Define

$$p_m(s) = P_m(s)/G_m \tag{9}$$

where $P_m(s)$ is the probability that the system is in state m at time $s\tau$ and $p_m(s)$ is the ratio of this probability to the number of microstates compatible with m. Our assertion that $S(s + 1) \geq S(s)$ is then equivalent to the assertion

$$\Sigma_m\, p_m\,(s + 1)\, G_m \ln p_m(s + 1) \leq \Sigma_m\, p_m(s)\, G_m \ln p_m(s). \tag{10}$$

The key to the proof is the observation [12] that the function $\varphi(x) = x \ln x$ is convex, which means that $\varphi\,(\Sigma_i\, q_i x_i) \leq \Sigma_i\, q_i\, \varphi(x_i)$ if $\Sigma_i\, q_i = 1$. Now our basic Eq. (1) can be rewritten in terms of the p_m to read

$$p_m(s + 1) = \frac{R + m + 1}{2R}\,\frac{G_{m+1}}{G_m}\, p_{m+1}(s) + \frac{R - m + 1}{2R}\,\frac{G_{m-1}}{G_m}\, p_{m-1}(s), \tag{11}$$

an equation which has the general form

$$p_m(s + 1) = \Sigma_l\, b_{lm}\, p_l(s) \tag{12}$$

where
$$\Sigma_l\, b_{lm} = 1, \tag{12'}$$

and where
$$G_m\, b_{lm} = G_l\, b_{ml} \tag{13}$$

Equations (12′) and (13) can be verified directly from the coefficients in Eq. (11).

Using the convexity of $x \ln x$ we obtain from Eq. (11),

$$p_m\,(s + 1) \ln p_m\,(s + 1) \leq \Sigma_l\, b_{lm}\, p_l\,(s) \ln p_l\,(s). \tag{14}$$

Multiply Eq. (14) by G_m and sum on m. We obtain

$$\Sigma_m\, G_m\, p_m\,(s + 1) \ln p_m\,(s + 1) \leq \Sigma_l\, p_l\,(s) \ln p_l\,(s)\, \Sigma_m\, b_{lm}\, G_m. \tag{15}$$

Using Eq. (13) and Eq. (12′) the second sum on the right hand side becomes

$$G_l\, \Sigma_m\, b_{ml} = G_l. \tag{16}$$

Hence Eq. (15) reduces to Eq. (10) which is our law for the monotonic increase of S. We see that S increases until the equilibrium distribution is reached, which happens eventually (as proved by Kac), and the entropy S then remains *constant* at its maximum value.

V. *Conclusion.* We have shown that the time dependence and the general behaviour of the entropy as defined in these two different ways are quite different. There is, of course, no contradiction between the two sets of results. Contradictions appear only if one is not careful to distinguish the sense in which the word entropy is used in the particular discussion. The purpose of this note was to prevent such confusion from arising again by discussing the entropy for the Ehrenfest model which is simple enough so the distinctions are completely transparent.

It is appropriate to conclude with some general remarks on therelationship between the two statistical theories of entropy discussed above and thermodynamics. Thermodynamics makes one clear statement about entropy which may be phrased as follows: an isolated system will always come to equilibrium and in doing so will always increase its entropy. Now it is well known that the very existence of fluctuation phenomena, typified by the Brownian motion, shows an incompleteness in the thermodynamic statement. The two statistical approaches to the entropy are two alternate ways of reformulating the Second Law of Thermodynamics so as to include the existence of fluctuations.

In the Boltzmann approach one keeps the idea of a single (macroscopic) equilibrium state and one admits forthrightly that there are violations of the Second Law, which becomes a statistical law. As we have seen in our example, every fluctuation from the equilibrium state is interpreted as a departure from equilibrium which decreases the entropy of the system, and such fluctuations, of arbitrarily large magnitude, are certain to occur. One saves the thermodynamic idea of *the* equilibrium state at the price of giving up the thermodynamic idea of this state as something achieved once and for all.

In the Gibbs approach the possibility of fluctuations is built, as it were, into one's concepts of entropy and equilibrium. The idea that a system comes to equilibrium now means not that it goes to a single state, but rather that the probabilities that the system is in any of its states take on particular values. In other words equilibrium is described in the language of probability, so that a system "in equilibrium" is actually moving from one state to another governed by the law determining the probability of finding it in any state. Correspondingly the entropy of the system, as we have seen, is a function of these probabilities and not of the actual state occupied, and this function monotonically approaches its maximum value, the entropy of the equilibrium distribution. In this approach the Second Law is kept as a rigorous statement but the concepts of equilibrium and entropy are made less intuitive.

Clearly either point of view is permissible and takes adequate account of the phenomena. One must sacrifice something either way since the simplicity of classical thermodynamics is inadequate for a description of a world which includes the Brownian motion.

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