CAN ENTROPY AND "ORDER" INCREASE TOGETHER?

P.T. LANDSBERG
Faculty of Mathematical Studies, University, Southampton, UK

Received 17 January 1984
Revised manuscript received 13 March 1984

Disorder and entropy are formally decoupled in such a way that it is possible for an expanding universe to have periods in which both entropy and order increase simultaneously. Some other consequences of this decoupling are traced and applications in statistical mechanics and to biological systems become possible.

Notable problems to which entropy concept has given rise include: (1) How can a structured or "orderly" universe have arisen from the initial hot big bang with a high degree of disorder and therefore presumably a large entropy. (2) How can additional "information", which is normally presumed to *lower* the estimate of the entropy of a system, sometimes *increase* it. An example of the latter situation occurs when a previously single energy level is found to be a doublet. The first problem has been discussed by cosmologists, most recently in refs. [1–3], by noting that the maximum entropy at any cosmological time may well increase faster than the actual entropy of the universe (or more precisely of the *model* universe). The second problem is related to questions of coarse-graining which have been much discussed for many years, see for example refs. [1,4].

Our purpose here is to decouple entropy and disorder. In *normal* thermodynamics where entropies, internal energies, etc. are extensive variables, this is easily achieved by defining disorder by [4]

$$D(n) = S(n)/k \ln n(t) , \qquad (1)$$

where n is the number of accessible microstates, $S(n)$ is the entropy of the system and k is Boltzmann's constant. The denominator is needed so that a doubled system, which has n^2 states, has the same disorder as the original system:

$$D(n^2) = S(n^2)/2k \ln n = D(n) . \qquad (2)$$

If we take the entropy as

$$S(n(t)) = -k \sum_{i=1}^{n(t)} p_i \ln p_i , \qquad (3)$$

where the p_i are the probabilities of the different states, then $S(n)$ has, for given $n(t)$, $k \ln n(t)$ as an upper bound, i.e. $D(n)$ is intensive, with

$$0 \leqslant D(n) \leqslant 1 . \qquad (4)$$

Thus "order" can be regarded as given by $1 - D(n)$. The key idea is that in actual situations $S(n)$ can increase with time *less* rapidly than $k \ln n(t)$. Hence order can increase and the time rate the change

$$\dot{D}(n) = [\dot{S}(n)/S(n) - \dot{n}/n \ln n]D(n)$$

can be negative, even though $\dot{S}(n)$ is positive. The new features arise from the variability of $n(t)$, which is considered a constant in normal theories.

We intend the disorder concept to be used with *any* of the usual statistical ensembles. Thus $p_i = 1/n(t)$ or $p_i = \exp(-E_i/kT)/Z$ in (3) leads to

$$S = k \ln n(t) \quad \text{or} \quad k \ln Z + U/T$$

which apply to the microcanonical and the canonical ensembles respectively with

$$Z \equiv \sum_{i=1}^{n(t)} \exp(-E_i/kT), \quad U \equiv \sum_{i=1}^{n(t)} p_i E_i .$$

In the former case $n(t)$ is the number of accessible

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(North-Holland Physics Publishing Division)

states at a given energy, in the second case $n(t)$ is the number of accessible states over a whole range of energies owing to a contact with a heat reservoir, provided only the number of particles is fixed. This latter restriction can also be removed by considering a p_i appropriate to the grand canonical ensemble. All of these possibilities, and others, are intended to be allowed for here.

A whole class of examples is furnished by biological systems where growth implies increasing $n(t)$, but they are not easy to quantify and such examples are not discussed here.

Example 1. This illustrates that information can *increase* entropy and also that it can change entropy and disorder in opposite directions. A system has two equally populated levels; the upper one is found to be a double level in a more accurate experiment. The probabilities go from $(\frac{1}{2}, \frac{1}{2})$ to $(\frac{1}{2}, \frac{1}{4}, \frac{1}{4})$ and the changes in entropy and disorder are respectively

$$k \ln 2 \to 1.5\, k \ln 2, \quad 1 \to 0.95\ (= 1.5 \ln 2/\ln 3).$$

Normally one thinks of "information" as *decreasing* entropies by virtue of the probabilities which were initially equal becoming unequal, it being assumed that $n(t)$ is unaffected. But here it is $n(t)$ which is adjusted.

Example 2. This illustrates that order can increase when entropy is constant. We adopt a Robertson–Walker model with a single cosmological fluid which satisfies $pV = gU$ where p, V are pressure and volume, U is the internal energy and g is a constant. For black-body radiation $g = \frac{1}{3}$. The Einstein equations show that the entropy of a comoving volume, and therefore UV^g, is time-independent. Thus (1) shows that disorder decrease or "order", $1 - D(n)$, *increases* even though entropy is constant. The reason is that for a given extent of the expansion [e.g. a given scale parameter $R(t)$] the number of accessible states can be taken as proportional to $R(t)^3$. But for the present example any positive power of R will do and then $n(t)$ increases while $S(n(t))$ remains constant.

Example 3. This illustrates that order and entropy can increase together. We adopt a two-fluid oscillating cosmological model in which there are long periods of only slowly increasing entropy [5,6]. For the observable universe $n(t) \propto (ct)^3$ and eq. (1) gives decreasing disorder so long as S increases less rapidly than $3k \ln t$. If a typical comoving volume is considered, $n(t) \propto R(t)^3 \propto t^{3/(q+1)}$ where we have assumed for simplicity a constant deceleration parameter $q \equiv -\ddot{R}R/\dot{R}^2 (> -1)$. In either case eq. (1) yields

$$D = \frac{S(t)/k}{a + b \ln t}$$

and as long as the entropy does not increase too fast, "order" increases as well. Here a is a constant and b is $3/(q+1)$. For a survey of recent estimates of q see ref. [7].

So far it has been assumed that the system obeys normal thermodynamics. It was therefore possible to have for the number $n_N(t)$ of states of a N-particle system

$$n_N(t) = n_1(t)^N,$$

whence

$$n_{2N}(t) = n_1(t)^{2N} = n_N(t)^2,$$

as used in (2). If the entropy is non-extensive, as it is for black holes, (2) fails. Let (1) be replaced by

$$D = S/S_{\max}, \tag{5}$$

provided S and $S_{\max}$ refer to the *same equation of state.* Then if, for example, $S \propto M^2$, as in black holes, then also $S_{\max} \propto M^2$, and D remains intensive and subject to (3). One can then again regard $1 - D$ as a measure of order which is intensive and (1) becomes a special case of (5). This shows also that disorder decreases whenever $S_{\max}$ increases sufficiently rapidly.

Example 4. If a cavity of adjustable radius R contains energy E and if only a black hole of mass M makes a significant contribution to the entropy, then from the Bekenstein–Hawking entropy formula [8,9] the maximum entropy of the system,

$$S_{\max} = 4\pi GkM^2/\hbar c = 2\pi kRE/\hbar c, \tag{6}$$

corresponds to all of the energy being in a black hole. We have used $2GM/R = c^2$ or

$$2GM^2/R = E. \tag{7}$$

From (5) and (6) one finds a noncontroversial example of the Bekenstein inequality [10]

$$S/E \leqslant 2\pi kR/\hbar c$$

for the black hole case. (How general it is a more controversial question, but the answer to it is not needed here.) We merely note that (5) yields a measure of disorder for this system, namely

$$D = (M_{bh}c^2/E)R_{bh}/R ,$$

where R, E refer to the cavity and the suffix bh refers to the black hole. The maximum can be attained only if E and R are related by (7).

If S in (5) were to be used for a gas of particles or photons (extensive) and S_{max} for a black hole system (nonextensive), D in (5) would cease to be an intensive variable. That problems arise from nonextensivity has been discussed elsewhere [11].

In more standard situations than those considered here, in which $n(t)$ is time *independent*, D and S will increase in proportion to each other. This holds in many cases (in fact, the usual cases) in statistical mechanics.

A more detailed estimate of "order" and entropy as a function of time based on various cosmological models will be given in due course.

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