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A deterministic entropy to monitor the evolution of microscopically simulated far-from-equilibrium structures

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Abstract

The cosmos seems live on entropy according to Boltzmann. Prigogine calls "live" structures like stars, flames and organisms "dissipative structures". A new functional of the microstate of realistic computer-implementable far-from-equilibrium systems is explained in its geometric and intuitive content. It can be combined with an exactly invertible algorithm to reveal the essence of a microscopically described system's inexorable approach towards equilibrium. All life-like roundabout ways can for the first time be studied in detail both forwards and backwards in time, so that their secret can be lifted.

Why should one take up a thread of thinking that was largely abandoned since Boltzmann's time—to understand in microscopic detail the approach towards equilibrium of a macroscopic gaseous or fluid or plasmatic system? The answer would be that the "core" of this mysterious engine of evolution has never been laid bare and made palpable up to the present moment.

In the following, we present a new attempt based on a technical improvement of an idea of Boltzmann's, namely, his famous H-function (originally pronounced ETA-function). In 1898, Boltzmann saw a way to define a deterministic microscopic entropy valid close to equilibrium [1]. His seminal idea was the following: Replace the N-particle system by $\underline{N}$ overlayed one-particle systems—so as if each particle were alone. Then look only at the differences between the state points of neighbouring particles. Boltzmann himself only looked at the momentum subspace. As the system of particles approaches equilibrium, the mean value, taken over all the individual differences, becomes a maximum. The same fact still holds true for the logarithm of the same sequence of mean values obtained on the way towards equilibrium. The absolute value of the resulting function, which becomes maximal at equilibrium, is nothing but the negative of the H-function; its positive obviously qualifies as a deterministic entropy, valid close to equilibrium.

The H-function method just described works satisfactorily only close to equilibrium [2]. The reason has to do with the fact that only next-neighbor distances were taken into account. Moreover, only the velocities (momenta), not the positions, were included as mentioned. Is it possible to do away with these shortcomings and arrive at a "more powerful" deterministic entropy function which remains valid arbitrarily far away from equilibrium?

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The following function appears to be up to the task:

$$S = k\left\{ \ln N + \frac{1}{N^2}\left[\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} \ln\left(\frac{1}{2}\pi^2 r_{ij}^4\right)\right]\right\}. \quad (1)$$

In Eq. (1), N is the number of particles and the r_{ij} are the momentary distances between *all pairs* of particles, in the full one-particle phase space into which all particles are projected, in accordance with Boltzmann's idea. [1] The formula (1), in the form written above applies to a gas in two dimensions. The second term on the right-hand side, the one within the straight vertical brackets, resembles a correlation function. While Eq. (1) itself has already been reported in Ref. [3], our aim here is to explain how it works in geometric and intuitive terms.

The main result of our previous publication is summarized in Fig. 1. Fig. 1 shows the approach to equilibrium in a 2-D volume of 100 particles whose positions had initially been confined to one half of the square (where they had been equidistributed). The approach towards the maximum is surprisingly smooth and monotonic—despite the small number of particles (100) involved. Is it possible to explain in simple terms how the new function (Eq. (1)) works?

To answer this question, let us first look at a simplified special case in one spatial dimension. In Fig. 2, only the particles' positions are presented. One sees three particles at a (near) maximal mutual spacing in a one-dimensional volume. For each particle, two distances exist with respect to the other particles (in the N-particle case, it is $N-1$ such distances). Their products form three rectangles as shown in the figure. The geometric mean taken over the three rectangles of Fig. 2 evidently generates a mean area—a mean two-dimensional cross-section through three-dimensional configuration space. This cross-section clearly is maximal for the configuration shown. The example allows us to get a geometric intuition into the workings of Eq. (1).

To this end, we now switch to configuration space. The configuration space of the three particles of Fig. 2 is depicted in Fig. 3. (Note that the position of each particle along the one-dimensional real space can indeed be read off from a single point now, since the cubic configuration space is made up of three orthogonal copies of the original space.) If we assume in the following that the three particles are equal, the cubic configuration space decomposes into six ($N!$) equal subspaces. This is shown in Fig. 3b which displays one of the six simplices formed [4]. The surviving subspace resembles a slightly tilted piece of Black-Forest Cherry Cake: The state point seen in Fig. 3b is the cherry.

The position of the dot in Fig. 3b corresponds to the particle configuration of Fig. 2. The bold arrow in Fig. 3b marks the distance of this state point from the base line of the simplex—which in turn corresponds to the main space diagonal of the original cube. The length of the arrow is an intuitive measure of the momentary volume of configuration space. More precisely, the arrow marks the "thickest orthogonal cross-section" through the simplex (namely, orthogonal to the base line). This principle carries through, as is shown in Fig. 4. As the number of particles is increased, in every case an equidistant configuration causes the distance of the state point from the hyperdiagonal to be near-maximal.

Specifically, if N is equal to 4, the simplex of Fig. 4b applies. It represents a segment of a tessaract (the unit cube in four dimensions). It possesses a l/24th (1/4!) of the latter's volume. In general, with N particles, we have the so-called "standard $N!$ triangulation of the N-cube" [5]. In each case, a state point characterized by a (near-) maximal "diameter" of configuration space (more precisely, a near maximal cross-section) is obtained. Always, the "waist-line" of the surviving simplex of configuration space contains the cherry. The cherry is the state point that is distinguished by all particles assuming a maximal distance from each other.

Fig. 4c exhibits one more innocent-looking feature. The decay towards the ends of the main diagonal of the cube (base line of the simplex) is concave rather than convex because the "orthogonal cross-section through phase space" decays more rapidly than its height (the radius of Fig. 3b). In fact, this decay is basically exponential. Note that in high dimensions, the outer regions (slices through the hyper-simplex away from the middle) contain virtually no volume any more, as has been worked out for a related case by Fields medalist Michael Gormov (Andreas Knauff, private communication 1998).

We now suggest that Eq. (1) works in general in exactly the same fashion as we have shown above for a special case (namely, for the configuration space of a one-dimensional gas). This leads us naturally to the conclusion that a momentary state point can indeed represent the instantaneously valid phase space volume.

[1] We shall see later that the product of these distances (the sum of their logarithms in Eq. (1)) actually represents a "mean diameter" in full phase space.

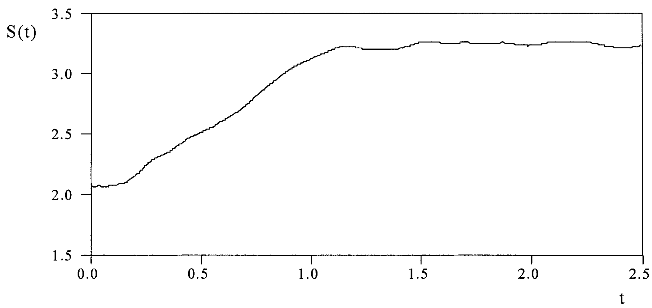

Fig. 1. Time-dependent entropy: Approach towards equilibrium from a far-from-equilibrium initial condition. Newtonian molecular dynamics simulation (MDS) of a 100-particle gas in two dimensions, with the equal particles initially confined to the left half plane. The function shown on the ordinate is defined by Eq. (1) (cf. text).

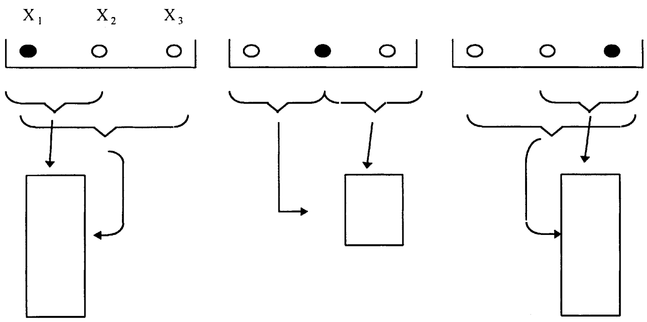

Fig. 2. Demonstration of how a mean phase space cross-section is constructed by Eq. (1). A simplified special case is shown: three particles in one dimension (cf. text).

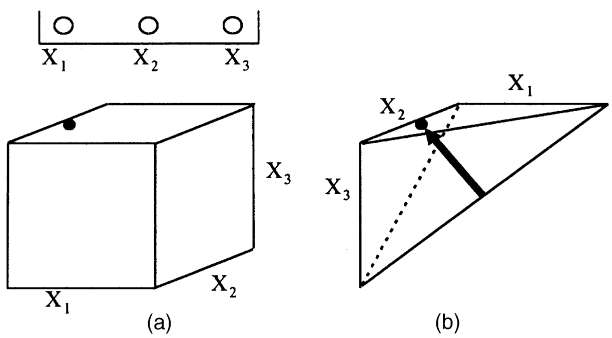

Fig. 3. The configuration space corresponding to the system of Fig. 2. (a) State point in full configuration space. (b) State point in the reduced configuration space valid in the presence of indistinguishability (cf. text).

We are now in the position to finally draw a connection to the famous Gibbs equilibrium entropy formula [6]. It reads

$$S_{eq} = k \ln \Phi. \tag{2}$$

In Eq. (2), Φ is the phase space volume at equilibrium (i.e., the maximum possible extension of phase space in all directions, taken in dimensionless units). We specifically propose that Eq. (1) can be interpreted as a time-dependent analog to Eq. (2). In the same vein, Eq. (2) becomes the $t \to \infty$ limit of Eq. (1). All that is still wanting is the correct normalization (which is deferred to a subsequent publication).

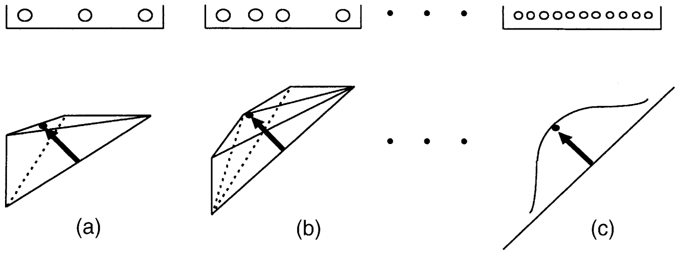

Fig. 4. Extension of Fig. 3 to arbitrary particle numbers. (a) “Cherry cake”, (b) “Hypercake”, (c) “Sombrero galaxy” (cf. text).

Is the finding presented above surprising in its philosophy? We think it is not. Hurley [7], for one, said very similar things on the basis of qualitative “topological” arguments. Secondly, modern microscopic transport theory points in the same direction (Günter Radons, personal communication 1998). Nevertheless, the above geometric picture appears to be new. Briefly speaking, Eq. (1) represents an explicit observable that allows one to hold a close watch over a multiparticle system—all the way along its approach towards equilibrium. Such an observable and way of monitoring has, apparently, been lacking up till now. We predict that future microscopic studies of simple dissipative structures (cf. [8]), like an autocatalytic oxygen–hydrogen reaction [9] or an evolutionary chemical soup [10] or a turbulent jet stream, will elucidate in more detail why it is that nature craves macroscopic complexity. A candidate hypothesis is Prigogine’s principle of minimum entropy production [11]. While the latter is analytically valid only close to equilibrium [11], a generalization (“principle of self-inhibition of energy dissipation”), covering the whole evolutionary “second arrow” of the cosmos, appears to be admissible. This hyphothesis can be falsified for the first time now using the algorithm of Eq. (1).

To conclude, a new observable of microscopic phase space has been discussed. This observable enables one to monitor and better understand in detail the approach of a far-from-equilibrium system towards its bottom line. The origin and breakdown of dissipative structures in nature can be studied in its finegrained causation, if one is ready to confine oneself to a computer universe. [2] Hereby, a calculation of the underlying Hamiltonian dynamics with an exactly reversible algorithm [12–15] will make it possible to go back and forth along a single microtrajectory of the system at hand. In this way, it becomes possible to check why a particular step in the evolution of the system in question (like an analog to the origin of life) took place in the way it did in the first place. We feel the science of complexity has acquired an important new tool.

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References

[1] Boltzmann L. Lectures on gas theory (Vorlesungen zur Gastheorie). Leipzig: Ambrosius Barth; 1898.
[2] Haile JM. Molecular dynamics simulations: elementary methods. New York: Wiley; 1992.
[3] Diebner HH, Rossler OE. Z Naturforsch 1998;53a:1–10.
[4] Rossler OE, Hoffmann M. J Comp Chem 1987;8:510–5.
[5] Mara PS. J Combin Theory (A) 1976;20:170–7.
[6] Gibbs JW. Elementary principles in statistical mechanics. New Haven: Yale University Press; 1902.
[7] Hurley J. Phys Rev A 1980;22:1205–9.
[8] Nicolis G, Prigogine I. Self-organization in nonequilibrium systems. New York: Wiley; 1977.
[9] Heinrichs M, Schneider FW. Ber Bunsenges Phys Chem 1983;87:1195.
[10] Rossler OE. Z Naturforsch 1971;26b:741–6.

[2] It goes without saying that in our own universe, microscopic observables cannot as yet (and presumably forever) be observed in the detail necessary to qualify for an analogous explicit investigation. This makes the model approach an unrenounceable tool.

[11] Prigogine I. Ac Roy Belg Bull Classe Sci 1945;31:600.
[12] Diebner HH. Investigations of exactly reversible algorithms for dynamics-simulations (in German). Diploma Thesis in Physics. Tübingen: University of Tübingen; 1993.
[13] Levesque D, Verlet L. J Stat Phys 1993;72:519–37.
[14] Nadler W, Diebner HH, Rossler OE. Z Naturforsch 1997;52a:585–7.
[15] Diebner HH. Z Naturforsch 2000;55a:405–11.