Problems in the statistical theory of open systems: Criteria for the relative degree of order in self-organization processes

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The aim of this paper is to examine two problems in the statistical theory of open systems, namely, (1) the connection between statistical and dynamic descriptions of motion in open systems, and the constructive positive role of dynamic instability in atomic motion as a basis for kinetic equations and (2) the different criteria for the relative degree of order in nonequilibrium states of open systems, namely, K-entropy, the Lyapunov function, and the Boltzmann-Gibbs-Shannon entropy renormalized to given mean effective energy (S-theorem). It is shown that the S-theorem can be used to determine the relative degree of order from experimental data on empirical realizations of leading characteristics for different values of control parameters.

1. INTRODUCTION

The aim of this paper is briefly to examine a number of fundamental questions in the statistical theory of *open systems*. Self-organization processes[1–4] occupy a special place among the various processes that occur in such systems. To emphasize the special role of collective, i.e., cooperative, effects in self-organization processes, Haken introduced the term *synergetics* to represent the new unifying branch of science.[3,4] The basic problem in synergetics is to identify general ideas, methods, and relationships in self-organization processes encountered in different branches of science and sociology.

Many scientists have contributed to the evolution of the theory of self-organization (synergetics). They included Boltzmann and Poincare, who laid the foundations of statistical and dynamic descriptions of complex motions, respectively, A. M. Lyapunov, who was one of the creators of the theory of stability of motion, which is basic to the theory of self-organization, A. N. Kolmogorov, who, among other things, introduced the concept of metric entropy that plays a significant role in the theory of dynamic systems, and L. I. Mandel'shtam, A. A. Andronov, N. S. Krylov, L. D. Landau, Ya. B. Zel'dovich, and many many others. The contribution of Vladimir Ivanovich Vernadskiĭ must be particularly noted.

Although the theory of self-organization is now backed by a considerable literature, it has not as yet provided an unambiguous answer to the question as to what is self-organization. Actually, an answer to this question is not essential. What we need is to establish the criteria for the relative degree of order, or organization, of the various nonequilibrium states of open systems. Unless such criteria are available, we cannot answer the most basic questions or determine the very presence of self-organization.

One of the basic problems is to identify the interrelation between dynamic and statistical descriptions of complex motions in open systems. We begin the systematic presentation of our material by introducing the various necessary concepts.

2. CHAOS AND ORDER IN OPEN SYSTEMS. CONTROL PARAMETERS

The concept of "chaos" has played a very significant role already in the world picture of ancient philosophers, including the early Platonists. In physics, "chaos," "chaotic motion," and "order" are fundamental but, nevertheless, not defined with adequate clarity.

Actually, since the classical papers of Maxwell, Boltzmann, and Gibbs, the motion of atoms in statistical equilibrium has been referred to as *chaotic*. However, the word chaotic is also applied to highly nonequilibrium states, e.g., states encountered in noise generators, turbulent flows, and so on. The phrase "dynamic chaos" has been widely adopted. It refers to complex motion in low-dimensional "simple" nonlinear dissipative dynamic systems. The classical example of systems of this kind is provided by the Lorenz equations of the theory of thermal convection.[5] A good description of the history of Lorenz's discovery is given in Ref. 6.

It is thus clear that the same word "chaos" is used to characterize very different types of complex motion, and this suggests that we must have criteria for the relative degree of order or disorder. These criteria include K-entropy (Krylov-Kolmogorov-Sinaĭ entropy), the Lyapunov indices, and the variously defined dimensions of the phase space of given types of complex motion. The theory of dynamic chaos has already attracted an extensive literature.[7–29]

In this paper, we shall devote considerable attention to criteria based on the comparison of Boltzmann-Gibbs-Shannon entropies renormalized to a given *mean effective energy*, and also on the comparison of entropy production in stable and unstable states of open systems. These results are reviewed for the first time. We shall also give a comparative analysis of the different criteria of order.

2.1. Control parameters

The choice of control parameters in self-organization processes is usually based either on existing information on the system or on additional investigations of, for example, bifurcation diagrams. Of course, this may involve errors, so that the criterion for the relative degree of order must also be capable of monitoring the fact that the control parameters have been chosen correctly. There is a great variety of characteristics from which the control functions can be selected. Let us consider a few examples.

In classical and quantum generators, this means feedback or pump, i.e., external forces. In multistable systems, a particular stationary state can be selected by altering the initial conditions. "Slow" time, e.g., the time taken to ob-

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serve the recovery of a patient, can serve as a control parameter. In hydrodynamics, the Reynolds, Rayleigh, and Taylor numbers play the role of control parameters, depending on the type of flow. When several control parameters are available, a search for the most effective mode of self-organization can be made.

2.2. Physical chaos

Let $a = (a_1 \ldots, a_n)$ be a set of parameters adopted as the control parameters and let us select two states corresponding to $a = a_0$, $a = a_0 + \Delta a$. By definition, the self-organization process corresponds to $\Delta a \geqslant 0$, and we have

$$a = a_0 + \Delta a, \quad \Delta a_i > 0 \ (i = 1, 2, \ldots, n). \tag{2.1}$$

The state with $a = a_0$ will be referred to as the *state of physical chaos*. We shall adopt it as the "origin" for the degree of order. The word "physical" is introduced to emphasize the physical character of these criteria. The important point is that the state of physical chaos can be a significantly nonequilibrium state.

2.3. Evolution and self-organization

The concept of evolution is very general. For example, in physics, we consider evolution toward the equilibrium state, whereas in open systems we examine evolution to stationary states. Evolution may be looked upon as the formation of a sequence of new structures. According to Darwin, the formation of new structures in biology proceeds by natural selection.

The question now is: what is the connection between evolution and self-organization? When we speak of self-organization processes, we are concerned with processes in which more complex and more perfect structures arise (according to the above criteria).

This approach leads to the question: is the evolution process a process of self-organization? The answer is that it is not because there is no "internal tendency" toward self-organization in physical or even biological systems. Actually, evolution can lead to degradation. An example of this in physics is the transition to the equilibrium state which, according to Boltzmann and Gibbs, is the most chaotic. The degradation of structures is, of course, also possible in biology, e.g., in disadvantageous mutations. It is therefore clear that self-organization is only one of the possible paths of evolution.

The present state of biological evolution can be judged from published reviews and books.[30–32] We shall return to question of biological evolution later, when we consider how entropy can be used to characterize the degree of diversity that is necessary for natural selection in evolution. However, we begin with the criteria for evolution and self-organization in physical systems.

3. BOLTZMANN'S *H*-THEOREM AND GIBBS' THEOREM

3.1. Boltzmann's H-theorem

The letter H in this theorem refers to *heat*. This emphasizes that the theorem is concerned with the evolution of entropy in the establishment of *thermal equilibrium*. It was formulated and proved by Boltzmann who considered the example of a tenuous gas (perfect gas in the thermodynamic sense).

The proof of the H-theorem is based on a property of the Boltzmann collision integral I_B, namely, $\int \varphi(p)\, I_B\, dp \geqslant \varphi$ for $\varphi = -k \ln f$ subject to the condition that the gas particles do not leave the system. The result is usually written in the form

$$\frac{dS}{dt} \geqslant 0, \tag{3.1}$$

where the entropy is given by

$$S(t) = -k \int \ln f \cdot f \, dr \, dp.$$

The equals sign in the above expression refers to the state of equilibrium for which f_0 is the Maxwell distribution.

However, for our purposes, we shall require a somewhat different formulation of the H-theorem. This follows from (3.1) and involves other properties of the collision integral, namely, $\int \varphi(p) I_B dp = 0$ for $\varphi = 1, p, p^2/2m$, and reduces to the proposition that there exists a Lyapunov functional $\Lambda_s = S_0 - S(t)$ with the following properties:

$$\Lambda_S \equiv S_0 - S(t) = k \int \ln \frac{f}{f_0} \cdot f \, dr \, dp \geqslant 0, \quad \frac{d(S_0 - S)}{dt} \leqslant 0,$$
$$\langle H \rangle = \left\langle \frac{p^2}{2m} \right\rangle = \text{const}. \tag{3.2}$$

Hence it follows that the equilibrium state is stable and corresponds to maximum entropy S_0. In (3.2), we indicate that the mean energy of the tenuous gas remains constant during evolution to equilibrium. This is not an additional condition, but a natural property of the Boltzmann equation. However, it is precisely for this reason that *entropy* (and not some other characteristic of the system) is the Lyapunov functional.

3.2. Gibbs' theorem

Let us now consider an arbitrary system with the Hamiltonian $H(X)$. The equilibrium state is characterized by the Gibbs distribution

$$f_0(X) = \exp \frac{F_0 - H(X)}{kT}, \quad \int f_0 \, dX = 1. \tag{3.3}$$

Let $f(X,t)$ be an arbitrary distribution with the same normalization, but with the further restriction that the expectation value of the Hamiltonian is the same for the distributions f_0 and f, i.e.,

$$\int H f_0(X) \, dX = \int H f(X, t) \, dX. \tag{3.4}$$

We shall use S_0 and S to denote the entropies corresponding to the distributions f_0 and f, respectively. According to Gibbs' theorem (see Chapter 11 in Ref. 33 and Chapter 4 in Ref. 34)

$$S_0 - S = k \int \ln \frac{f}{f_0} \cdot f \, dX \geqslant 0. \tag{3.5}$$

Thus, if the mean energy is constant, the entropy is a maximum in the state of equilibrium. This does not involve any restriction on the interaction between particles in the system. In this respect, the Gibbs result is more general than the H-theorem. However, we are not concerned here with the temporal evolution of the function $S_0 - S(t)$ during relaxation to the equilibrium state.

4. *H*-THEOREM IN THE THEORY OF BROWNIAN MOTION

Consider the simple case in which Brownian particles are uniformly distributed in space. In the case of linear fric-

tion, the velocity distribution function is then the solution of the Fokker-Planck equation

$$\frac{\partial f(v,t)}{\partial t}=D\frac{\partial^2 f}{\partial v^2}+\frac{\partial}{\partial v}(\gamma v f),$$
$$D=\gamma\frac{kT}{m},\quad \int f\,dv=1. \tag{4.1}$$

The equilibrium solution, i.e., the Maxwell distribution, will be written in the form of (3.3):

$$f_0=\exp\frac{F_0-H}{kT},\quad H=\frac{mv^2}{2}. \tag{4.2}$$

For a system in a thermostat, we can determine the free energy for a nonequilibrium state[34,35]:

$$F(t)=U(t)-TS(t),\quad U(t)=\langle H\rangle,\quad S(t)=-k\int \ln f\cdot f\,dv. \tag{4.3}$$

The free energy difference $F(t)-F_0$ is a Lyapunov functional. The following inequalities are then satisfied (see Chapter 11 in Ref. 34):

$$\Lambda_F\equiv F(t)-F_0=kT\int \ln\frac{f}{f_0}\cdot f\,dv\geqslant 0,\quad \frac{d(F-F_0)}{dt}\leqslant 0. \tag{4.4}$$

In the theory of Markov processes,[36,37] the Lyapunov functional Λ_F is called the *Kullback entropy*.

We have thus arrived at a result that is analogous to the Boltzmann H-theorem, but with the significant difference that, in the case of Brownian motion, the Lyapunov function is replaced with the free energy of the nonequilibrium state. On the other hand, free energy differs from entropy in that it cannot be defined for an arbitrary nonequilibrium state and does not have the complete set of properties that are essential as a measure of indeterminacy in the statistical description.

In Brownian motion, entropy can also play the part of the Lyapunov functional. However, this requires a renormalization of the solution of (3.1) to a given mean energy $\langle E\rangle=\langle mv^2/2\rangle$ [cf. (3.2) and (3.4)]. If we now use $\tilde{S}(t)$ to denote the entropy determined by the renormalized distribution, the Lyapunov functional $\tilde{\Lambda}_S=S_0-\tilde{S}(t)$ will satisfy (3.2). For equation (1), we can write our results in the explicit form

$$S_0-\tilde{S}(t)=\frac{3}{2}k\ln\frac{T(t)}{T_0}\geqslant 0,$$
$$\frac{d(S_0-\tilde{S})}{dt}=-3k\gamma\frac{T(t)-T_0}{T(t)}e^{-2\gamma t}\leqslant 0. \tag{4.5}$$

The relationship between the initial, current, and "final" (thermostat) temperatures [T_0, $T(t)$, and T, respectively] follows from the additional condition $\langle E\rangle=\langle mv^2/2\rangle$ and takes the form

$$\frac{m\langle v\rangle^2}{2}+\frac{3}{2}kT(t)=\frac{3}{2}kT,\quad T_0\leqslant T(t)\leqslant T. \tag{4.6}$$

In the theory of Brownian motion, the above renormalization is possible only in a limited range of initial velocities, so that the above example is, of course, only illustrative. It is nevertheless useful because it demonstrates that, at least in principle, the entropy Lyapunov functional $\tilde{\Lambda}_S$ can also be used for a system in a thermostat. When we formulate the criteria for the relative degree of order, i.e., the self-organization criteria, we shall see that this possibility is constructive. Before we go any further, let us examine the more complicated example of Brownian motion in an open system.

5. *H*-THEOREM. BROWNIAN MOTION IN THE VAN DER POL OSCILLATOR

We shall use the Fokker-Planck equation for the energy distribution function describing oscillations in the Van der Pol oscillator (see Section 6 of Chapter 12 in Ref. 34):

$$\frac{\partial f(E,t)}{\partial t}=D\frac{\partial}{\partial E}\left(E\frac{\partial f}{\partial E}\right)+\frac{\partial}{\partial E}[(-a+bE)Ef]; \tag{5.1}$$

where D is a given noise intensity, $a=a_p-\gamma$, a_p is the feedback (pump) parameter, and γ, b are the linear and nonlinear friction coefficients. The stationary solution of (5.1) is

$$f_0=\exp\frac{F_0-H(E)}{D},$$
$$H(E)=-aE+\frac{1}{2}bE^2,\quad \int_0^\infty f\,dE=1; \tag{5.2}$$

where $H(E)$ represents the effective Hamiltonian and F_0 is the corresponding free energy. For nonequilibrium states

$$F(t)=\langle H\rangle-DS,$$
$$S(t)=-\int \ln f(E,t)\cdot f(E,t)\,dE. \tag{5.3}$$

The Lyapunov functional is again given by the difference between free energies (see Chapter 12 and Ref. 34 and also Ref. 35):

$$\Lambda_F=F(t)-F_0=D\int \ln\frac{f(E,t)}{f_0}\cdot f(E,t)\,dE\geqslant 0,$$
$$\frac{d|F(t)-F_0|}{dt}\leqslant 0. \tag{5.4}$$

We shall now show that the H-theorem can also be formulated for entropy. We again introduce renormalization, but now for a given value of the function $H(E)$:

$$\int H(E)\tilde{f}(E,t)\,dE=\int H(E)f_0(E)\,dE. \tag{5.5}$$

The renormalized noise intensity $\tilde{D}\{\tilde{f}\}$ is found from this equation. It depends functionally on the distribution $\tilde{f}$ that satisfies the nonlinear Fokker-Planck equation with the diffusion coefficient[38] $\tilde{D}\{\tilde{f}\}$. The Lyapunov functional $\tilde{\Lambda}_S$ is determined by the entropy difference $\tilde{S}(t)$, S_0 and satisfies the inequalities

$$\tilde{\Lambda}_S=S_0-\tilde{S}(t)=\int_0^\infty \ln\frac{\tilde{f}(E,t)}{f_0}\cdot\tilde{f}(E,t)\,dE\geqslant 0,$$
$$\frac{d(S_0-\tilde{S})}{dt}\leqslant 0,\quad \langle H(E)\rangle=\text{const}. \tag{5.6}$$

We thus see that the renormalized entropy $\tilde{S}(t)$ increases during evolution to the stationary state with the distribution $F_0(E)$, and remains constant when the stationary state is reached.

We note once again that the use of entropy as the Lyapunov function has definite advantages. First, entropy can be expressed in terms of the distribution function for an arbitrary nonequilibrium state for which a distribution function can be defined. Second, in contrast to entropy, free energy does not have a set of properties that could be used as a measure of indeterminacy or chaos.

The increase in entropy (or reduction in free energy) in open systems undergoing evolution to a stationary state is

possible because the given parameters a, b, and D are sufficient to determine only the stationary state, i.e., we are free to choose the initial distribution $f(E,t=0)$.

6. EVOLUTION IN THE SPACE OF CONTROL PARAMETERS. THE S-THEOREM

We now turn to one of the basic problems in the statistical theory of open systems, i.e., the formulation of criteria for the relative degree of order in nonequilibrium states in the space of control parameters. We must first select the parameters that we shall adopt as control parameters (see Section 2). We recall that these parameters may include the "slow" time that characterizes, for example, the time of recovery of a patient. For the Van der Pol oscillator, it is natural to take the feedback (pump) parameter a_p as the control parameter.

We shall assume that the control parameters vary so slowly that each intermediate state is a stationary state and can be characterized, for example, by a distribution $f_0(E,a)$ [see (5.2)]. We can then speak of the evolution of stationary states in the space of control parameters.

As in Section 2, we select two states with $a=a_0$, $a=a_0+\Delta a$. The former is taken as the state of "physical chaos" and $f_0(X,a_0)$ is the corresponding distribution function. Let us write the latter in the form of the canonical distribution (if this is impossible, we use the scheme presented in Section 7):

$$f_0(X,\ a_0)=\exp\frac{F_0-H(X,\ a_0)}{D},\qquad \int f_0\,\mathrm{d}X=1, \tag{6.1}$$

where $H(X,a_0)$ is the effective Hamiltonian [compare this with (5.2)]. In addition to f_0, we also introduce the distribution function $f(X,a_0+\Delta a)$ which corresponds to $a=a_0+\Delta a$:

$$f=f(X,\ a_0+\Delta a),\qquad \int f\,\mathrm{d}X=1,\qquad \Delta a\geqslant 0. \tag{6.2}$$

Let us now compare the entropies S_0, S for the states a_0, $a_0+\Delta a$, subject to the additional condition that $H(X,a_0)$ is constant:

$$\int H(X,\ a_0)\,\tilde f_0\,\mathrm{d}X=\int H(X,\ a_0)\,f(X,\ a_0+\Delta a)\,\mathrm{d}X. \tag{6.3}$$

The renormalized distribution will be written in the form

$$\tilde f(X,\ a_0,\ \Delta a)=\exp\frac{\tilde F_0-H(X,\ a_0)}{\tilde D(\Delta a)},\qquad \int \tilde f_0\,\mathrm{d}X=1. \tag{6.4}$$

The function $\tilde F_0(\tilde D)$ follows from the normalization condition for $\tilde f_0$. The renormalized quantity $\tilde D$ can be found from (4):

$$\tilde D=\tilde D(\Delta a),\qquad \tilde D(\Delta a)|_{\Delta a=0}=D; \tag{6.5}$$

where $\tilde S_0$ is the entropy of the renormalized state. We then have the inequality

$$\tilde S_0-S=\int \ln\frac{f}{\tilde f_0}\cdot f\,\mathrm{d}X\geqslant 0\quad \text{for}\quad \langle H(X,\ a_0)\rangle=\text{const}. \tag{6.6}$$

The change in the degree of order accompanying the transition $a_0\to a_0+\Delta a$ will depend on the form of the solution of (3). If

$$\tilde D(\Delta a)>D, \tag{6.7}$$

i.e., if the system with $a=a_0$ must be "heated" to satisfy (6.3), the $a_0\to a_0+\Delta a$ transition proceeds from a less ordered to a more ordered state. The entropy difference (6.6) then serves as a quantitative measure of the increase in the degree of order.

If the inequality (6.7) is not satisfied, i.e., $\tilde D(\Delta a)<D$, the change $\Delta a>0$ is not a control parameter. The search for new control parameters can then be continued.

The above conclusion that the state with $a=a_0+\Delta a$ has a higher degree of order when (6.7) is satisfied can be confirmed as follows. Let us adopt the state with $a_0+\Delta a$ as the state of physical chaos, and solve the corresponding equation (6.3). If it turns out that $\tilde D(\Delta a)<D$, the above conclusion that the state with $a=a_0$ is the state of higher degree of order can be regarded as confirmed. On the other hand, if $\tilde D(\Delta a)>D$ for this inversion, the increase in the degree of order occurs toward the larger of the two values $\tilde D(\Delta a)-D$ for both forward and reverse transitions.

Definite information on the evolution of close nonequilibrium states can be obtained by analyzing the Lyapunov function for $\Delta a\ll a_0$, a. This can be done by using (6) and the derivative of Λ_0 with respect to Δa. If

$$\frac{\mathrm{d}\Lambda_S}{\mathrm{d}\Delta a}\geqslant 0 \tag{6.8}$$

and, consequently, the signs of (6) and (8) are the same, the change Δa is a control parameter.

Let us now consider a simple illustrative example of the application of the S-theorem. In particular, let us use this criterion to compare the degrees of order of the following Maxwell distributions ($m=1,k=1$):

$$f_0=\frac{1}{(2\pi T_0)^{1/2}}\exp\left(-\frac{v^2}{2T_0}\right),$$

$$f_1=\frac{1}{(2\pi T_1)^{1/2}}\exp\left[-\frac{(v-u)^2}{2T_1}\right]. \tag{6.9}$$

The state labelled 0 is taken as the chaotic state, whereas state 1 has nonzero mean velocity. We now perform the renormalization $f_0\to\tilde f_0$. The new temperature $\tilde T\equiv\tilde D$ can be found from (3). This specifies the heating condition indicated by the inequality (7):

$$\tilde T=T_1+u^2>T_0. \tag{6.10}$$

The entropy difference $\tilde S_0$, S can now be found from (6). This yields

$$\tilde S_0-S=\frac{1}{2}\ln\frac{\tilde T}{T_1}=\frac{1}{2}\ln\frac{T_1+u^2}{T_1}\geqslant 0. \tag{6.11}$$

Let us begin with the special case for which $u=0$ and, consequently, the entropy difference in (11) is zero. This means that, according to the criterion provided by the S-theorem, the degree of order, i.e., the structural complexity of the distributions f_0 and f, determined by symmetry, is the same. The states 0 and 1 are, of course, still different. The difference may be revealed by other criteria, e.g., by the Shannon entropy (information content) [see also (11.5)], and also by the values of the Lyapunov function (4.4), i.e., the Kullback entropy.

It follows from (10) and (11) that, when $u\neq 0$, state 1 is the more ordered one. This may appear to be a paradoxical conclusion when $T_1>T_0$ and f_1 is the broader distribution. However, in accordance with the S-theorem and, indeed, according to common sense, the higher degree of order of

state 1 for $u^2 > 0$ is due to the following.

When $u \neq 0$, the symmetry of the distributions f_0 and f_1 is lost and f_1 becomes structurally richer. Even for small values of u^2, this is a qualitative change because it reveals the possibility of a "forward" motion of the system as a whole. This possibility persists for any ratio of T_0 and T_1.

More substantive examples will be considered below. Here, we merely note that the first calculations of the relative degree of order of nonequilibrium states, based on the values of renormalized entropy, were reported in Refs. 39 and 40. The proposition formulated in these papers was referred to as the S-theorem (the letter S refers to *self-organization*). This emphasizes that we are indeed dealing with a criterion for self-organization. Early work is reviewed in Ref. 41 and a more general proof is given in Ref. 42. Further developments are reported in Refs. 53, 57, and 74.

7. COMPARISON OF THE RELATIVE DEGREE OF ORDER IN OPEN SYSTEMS, USING THE *S*-THEOREM AND EXPERIMENTAL DATA

Before the above criterion can be used for practical purposes, we must have information on the structure of the effective Hamiltonian. This can be obtained from a mathematical model of the system under consideration. However, the construction of a mathematical model of an open system is often found to encounter considerable difficulties. It is therefore important to be able to estimate the relative degree of order directly from experimental data. This can be done as follows.[43] Let a represent an internal parameter characterizing the system under consideration. The first step is to obtain two realizations of our process $X(t,a_0)$, $X(t,a_0+\Delta a)$ for two values of the control parameter $a = a_0$, $a = a_0 + \Delta a$. If the realizations are long enough, we can find the distributions

$$f_0 = f_0(X,\ a_0), \quad f = f(X,\ a_0 + \Delta a). \tag{7.1}$$

normalized to unity. We shall assume that Δa is a control parameter. We take the state with $a = a_0$ as physical chaos and use f_0 to define the effective Hamiltonian

$$H_{\text{eff}}(X,\ a_0) = -\ln f_0(X,\ a_0). \tag{7.2}$$

This terminology is justified by the fact that the distribution $\tilde{f}_0$ renormalized to the $\langle H_{\text{eff}}\rangle$ will take the form of a canonical Gibbs distribution with the "Hamiltonian" H_{eff}.

It follows from (2) that, to find the function H_{eff}, we need not have additional information other than a knowledge of the realization from which the form of the distribution f_0 is determined.

We shall write the renormalized function in the form of

$$\tilde{f}_0(X,\ a_0,\ \Delta a) = \exp\frac{F - H_{\text{eff}}(X,\ a_0)}{D(\Delta a)}, \quad \int \tilde{f}_0\,\mathrm{d}X = 1. \tag{7.3}$$

The dependence of the "free energy" F on the effective temperature D will be defined by the normalization condition for $\tilde{f}_0$, and the dependence of D on Δa by the solution of the equations [cf. (6.3)]

$$\int H_{\text{eff}}(X,\ a_0)\tilde{f}_0(X,\ a_0,\ \Delta a)\,\mathrm{d}X = \int H_{\text{eff}}(X,\ a_0)\,f(X,\ a_0+\Delta a)\,\mathrm{d}X. \tag{7.4}$$

This gives us the function $D(\Delta a)$ such that

$$D(\Delta a)|_{\Delta a=0} = 1. \tag{7.5}$$

As before, we use the distributions $\tilde{f}_0$, f to find the entropy difference

$$\tilde{S}_0 - S = \int \ln\frac{f}{\tilde{f}_0}\cdot f\,\mathrm{d}X \geqslant 0 \quad \text{for} \quad \langle H_{\text{eff}}\rangle = \text{const}. \tag{7.6}$$

If the solution (5) of (4) is such that

$$D(\Delta a) > 1, \tag{7.7}$$

the state with $a = a_0 + \Delta a$ is more ordered than that adopted as physical chaos. The entropy difference (6) serves as a quantitative measure of the increase in the degree of order. To confirm the validity of this conclusion, we can use the scheme indicated at the end of the last Section.

Let us now return to the example considered at the end of Section 6. Let us suppose that the distributions (1) obtained from experimental data have the form given by (6.9). Using the procedure presented in this Section, we find that the function $D(\Delta a)$ is given by $D = (T_1 + u^2)/T_0$ and, consequently, inequality (7) is identical with (6.10). The expression given by (6.11) is also found to remain in force, as are all the conclusions drawn earlier.

We must now compare our criterion with other criteria for the relative degree of order. However, we must first examine some general questions in the statistical theory of open systems.

8. DYNAMIC AND STATISTICAL DESCRIPTION OF OPEN SYSTEMS

We shall divide systems into dynamic and statistical (stochastic). This subdivision is not generally accepted. For example, the well-known paper by Sinai[6] has the title "Stochasticity of dynamic systems." The phrase "chaotic motion of determined dynamic systems" is extensively used in Ref. 22.

We shall base our subdivision into the above two classes on a numerical experiment. The classification will be founded on the *reproducibility of motion* from given initial data. By definition, *dynamic* motions are *reproducible* and *stochastic* (statistical) motions are *irreproducible* from initial data in dissipative systems.

Naturally, in real systems, in which noise is unavoidable, all processes are to some extent statistical. On the other hand, in a statistical experiment with dynamic dissipative systems, the initial conditions can be accurately repeated (within the given limits of precision). The reproducibility of solution then depends on the structure of the mathematical model. If the equations do not contain random sources, the process is reproducible and motion is dynamic although it can be unpredictable because of its complexity. The following points must be borne in mind when statistical processes are investigated in numerical experiments.

The random number generators used in computer systems rely on particular algorithms and are therefore deterministic. However, they can be regarded as random if the characteristic repetition time is much greater than the characteristic relaxation times of the dynamic systems under consideration.

Complex motions in dynamics were first discovered in Hamiltonian systems and the phrase "dynamic chaos" was introduced for them. At present, it is widely used to charac-

terize complex motions in dissipative dynamic systems. We must now examine the basic characteristic features of dynamic chaos.

K-entropy. Lyapunov indices. The principal feature of dynamic chaos is the dynamic instability of motion, i.e., the exponential divergence of initially close trajectories.

K-entropy (Krylov-Kolmogorov-Sinai entropy) is a measure of this exponential divergence. It is related to the mean rate of divergence of initially close trajectories and, consequently, to the Lyapunov indices. It is expressed in terms of the positive Lyapunov indices λ_i by the Pesin formula (see Refs. 12 and 24)

$$K = \sum_i \lambda_i, \quad \lambda_i > 0. \tag{8.1}$$

When positive indices λ_i are absent, we have $K = 0$.

The Lyapunov indices of nonlinear dissipative open systems are determined from numerical experiments. For example, for the one-dimensional logistic equation in discrete time

$$x_{n+1} = f(x_n), \quad f(x) = (a - x)\,x, \quad 0 \leqslant x \leqslant 4, \quad 0 \leqslant a \leqslant 4, \tag{8.2}$$

the entropy is $k = \lambda$ and the Lyapunov index is given by

$$\lambda = \lim_{n \to \infty} \frac{1}{n} \sum_{i=0}^{n-1} \ln \left| \frac{\partial f}{\partial x} \right|_{x_i}. \tag{8.3}$$

This expression for λ can be taken as a definition. Its derivation in Ref. 12 from the original equation (2.7) is not entirely satisfactory because, in the numerical experiment, the mean separation between trajectories is finite and if the attractor is finite, the quantity λ given by (2.7) in Ref. 12 must be zero. This also applies to formula (5.15) in Ref. 12, which gives the Kolmogorov entropy.

Thus, (3) can be adopted as the definition of K-entropy and the Lyapunov index for one-dimensional motion. Significantly, it takes into account only the divergence of trajectories over a unit step for zero initial separation for *each step*. This means that it takes into account only local nonlinearity. We shall return to this question in Section 16.

Mixing in phase space is a consequence of the exponential divergence of initially close trajectories, i.e., the dynamic instability of motion. The role of mixing in the justification of the statistical theory was identified by N. S. Krylov.[44]

There are also other characteristics of dynamic chaos (continuity of spectrum, finite correlation time), but they are consequences of dynamic instability for which the criterion is positive K-entropy.

We now face an important question: to what extent is the designation "dynamic chaos" justified, bearing in mind that the complex motion that represents dynamic chaos is reproducible in numerical experiment?

The question is sensible in another respect as well. We shall see in the next Section that exponential divergence and mixing can play a constructive and positive role in the statistical theory of nonequilibrium processes. We must now explain the significance of this statement which seems paradoxical at first sight.

9. CONSTRUCTIVE ROLE OF DYNAMIC INSTABILITY OF MOTION IN THE STATISTICAL THEORY OF NONEQUILIBRIUM PROCESSES

To illustrate the basic idea, we begin with a simple example from sociology. Let us imagine that an international congress has been taking place. The location of the attendees immediately after the closure procedure will be taken as the initial position. We shall consider two possible variants of subsequent motion of the attendees: (1) at the end of the congress, they move together without separating from one another and (2) the attendees depart to their respective homes and places of work, i.e., they separate exponentially. In other words, the motion of the attendees becomes "dynamically unstable." The question is: which of these two possibilities is more favorable to progress?

The first variant of motion is of course favorable over a limited interval of time because it preserves personal contact. Undoubtedly, however, it is the second variant that ensures a more extensive dissemination of information acquired during the meeting, i.e., it assists progress. The constructive, positive role of "dynamic instability of motion" is obvious in this case.

We also note that this type of "dynamic instability," i.e., the exponential divergence of the trajectories of attendees is planned by the organizing committee in advance: as a rule, the committee tries to provide the participants with return tickets.

We now turn to the statistical theory of nonequilibrium processes. We can consider four levels of approximation in the mechanics of continuous media: (1) the kinetic equations, (2) the hydrodynamic equations, (3) the reaction-diffusion equations, and (4) the equations of chemical kinetics.

The possibility of "downward motion" in this hierarchy of equations for the macroscopic characteristics is based on the use of the corresponding small parameters. Since the Boltzmann transport equation is the highest in this hierarchy, e.g., for tenuous gases, it is natural to try to demonstrate the constructive role of atomic motion in the dynamic instability of the gas when we justify the Boltzmann equation using the reversible equations of atomic motion based on the Hamilton equations.

Following the classical papers of Bogolyubov, Kirkwood, Born, and Green, the conditions for the validity of the Boltzmann transport equation were discussed by many authors. From our point of view, the only significant condition is the one that determines the possibility of an approximate representation of a tenuous gas by a continuous medium.

The one-component tenuous gas has only one small dimensionless parameter, i.e., the *density parameter* $\varepsilon = nr_0^3$. The relationships between the three characteristic length parameters, namely, the size of the atom r_0, the mean separation between the atoms r_{av}, and the mean free path $l \sim 1/nr_0^2$, can be expressed in terms of the density parameter. Let us now define infinitessimal elements of length (l_b) and time (τ_b). The corresponding volume will be denoted by V_b. The mean number of particles in V_b is then $N_b = nV_b$. The continuum approximation is possible if $N_b \gg 1$, whereas the kinetic description is possible provided $l_b \ll l$ and $\tau_b \ll \tau$. The quantities τ_b, l_b, V_b, N_b can be defined as follows[45–48,34]:

$$\tau_b = \varepsilon^{1/2}\tau \ll \tau, \quad l_b = \varepsilon^{1/2} l \ll l, \quad N_b = \frac{1}{\varepsilon^{1/2}} \gg 1. \qquad (9.1)$$

For example, at atmospheric pressure, we have $\varepsilon \sim 10^{-4}$, so that $N_b \sim 100$.

The Boltzmann transport equation and, consequently, the entire hierarchy of equations of continuum mechanics can usually be constructed for macroscopic functions without resorting to the concepts of dynamic instability, K-entropy, and mixing. However, the use of these concepts helps us to achieve a more complete understanding of the causes of irreversibility when transport equations are constructed on the basis of reversible equations of motion. The first significant steps in this direction were made by N. S. Krylov.[44] Much attention is devoted to these questions by Prigogine in his books.[2,58]

We must now establish the relationship between the minimum time for the development of dynamic instability in the motion of atoms and the time interval τ_b (Ref. 49). We shall take into account the fact that the instability development time for the motion of an individual atom is $\tau_{\text{instab}} \sim \tau$ (Ref. 50). Correspondingly, the characteristic instability development time for the motion of any (single) particle with the volume V_b is smaller by the factor N_b. This leads to the relationship[49]

$$(\tau_{\text{instab}})_b \sim \tau_b. \qquad (9.2)$$

The minimum characteristic time for the development of instability is of the order of τ_b. This is an additional argument in favor of the above definition of τ_b, but there is also another significant argument.

The dynamic instability of the motion of billiard-ball type atoms, which leads to mixing, facilitates the very possibility of a transformation from reversible microscopic equations of motion of atoms to the much simpler Boltzmann equation for the distribution function, which is smoothed over the volume V_b of microscopic phase density. This is in fact a manifestation of the constructive, positive role of the dynamic instability of the motion of gas atoms when the statistical theory is constructed.

The above discussion does not, of course, exhaust the problem of the role of dynamic instability in statistical theory. Actually, the instability manifests itself in the equations of macroscopic motion, as well, e.g., in the equations of hydrodynamics. This was first demonstrated by Lorenz[5] for the model equations describing thermal convection.

The above approach to the role of dynamic instability gives rise to the following question: can the dynamic instability of the motion of macroscopic characteristics (rather than of atoms) play a constructive role in evolution processes? Does it lead to chaos in open dissipative systems, or does it give rise to the possibility and development of self-organization? To answer these questions, we can use the criteria for the relative degree of order in open systems that were discussed above.

We shall apply these criteria to a number of examples in order to show that self-organization processes are possible even in the presence of the dynamic instability of the motion of macroscopic characteristics of open systems. However, we must first consider some further general questions in the statistical theory of nonequilibrium processes.

10. TIME AND PHASE AVERAGES AND THE GIBBS ENSEMBLE FOR NONEQUILIBRIUM PROCESSES. LOCAL ERGODICITY CONDITIONS

10.1. Dynamic and statistical distributions

We recall that, in Section 7, motion in dissipative nonlinear open systems was arbitrarily divided into dynamic and statistical. At any level of the theory, the dynamic description of dissipative systems corresponds to the zero-order approximation in fluctuations. This approximation is, however, often inadequate. For example, unless fluctuations are taken into account, it is impossible to provide a complete description of the crossing of bifurcation points in self-organization processes. Here we find a profound analogy with fluctuation processes in second-order phase transitions.

Fluctuations in nonequilibrium processes in dissipative systems can be taken into account at different levels of description, i.e., there is a hierarchy of fluctuation phenomena. For example, in the theory of Brownian motion, we can distinguish three levels of description, namely, (1) the description based on the dynamic equations, which is the zero-order approximation in fluctuations, (2) the Langevin equations with a random source, determined by small-scale fluctuations ($\tau_{\text{cor}} \ll \tau_{\text{rel}}$), and the corresponding equation for the distribution function, e.g., the Fokker–Planck equation that is the dynamic equation for the distribution function, and (3) the transport equation with the Langevin source, which can serve as the initial equation for the description of transport fluctuations in Brownian motion. In accordance with this hierarchy, we can introduce the three distribution functions

$$f^{(d)}(X,t), \quad f(X,t), \quad \tilde{f}(X,t) \qquad (10.1)$$

of which the first corresponds to the dynamic description, the second to the statistical description, but with a determined distribution function, and the third to the statistical description in which the distribution function is itself random.

Let us illustrate the foregoing discussion by considering the example of a mathematical model of the Van der Pol oscillator with symmetric nonlinearity. We shall use this model later as the basis for more complicated self-organizing systems. The equations for the oscillator are

$$\frac{dx}{dt} + \frac{1}{2}(-a + bE)x = v; \quad \frac{dv}{dt} + \frac{1}{2}(-a + bE)v + \omega_0^2 x = 0 \qquad (10.2)$$

where the energy of the oscillations is given by

$$E = \frac{1}{2}(v^2 + \omega_0^2 x^2). \qquad (10.3)$$

and ω_0 is the eigenfrequency. As in Section 3, $a = a_p - \gamma$, where a_p is the feedback (pump) parameter and γ, b are the linear and nonlinear coefficients of friction. A closed equation of energy then follows from (2). This equation and its solution take the form

$$\frac{dE}{dt} = (a - bE)E, \quad E(t) = E_0 \frac{a}{b}\left[E_0 - \left(E_0 - \frac{a}{b}\right)e^{-at}\right]^{-1}. \qquad (10.4)$$

This solution determines the solution of (2).

The following dynamic distribution corresponds to (2):

$$f^{(d)}(x,v,t) = \delta(x - x(t))\,\delta(v - v(t)). \tag{10.5}$$

If we introduce the δ-correlated Langevin source of given intensity D into the dynamic equations (2), we can transform from Langevin's equations to the Fokker-Planck equation for the distribution $f(x,v,t)$. The corresponding equation for the random distribution $\tilde{f}(x,v,t)$ can be used to calculate the kinetic fluctuations.

10.2. Gibbs ensemble in the theory of nonequilibrium processes. Time and phase averages

Let $A(X)$ be an arbitrary function of the set of dynamic variables X. We shall take the dynamic distribution in the form

$$f^{(d)}(X,t) = \delta(X - X(t)). \tag{10.6}$$

Naturally, the averaged functions $A(X)$ obtained with this distribution do not lead to smoothing. Smoothing is accomplished only by using the statistical distribution corresponding to the incomplete description instead of (6).

In the statistical theory of nonequilibrium processes, the incompleteness of description arises during smoothing (averaging) over a physically infinitesimal volume V_b or the corresponding time interval τ_b. This smoothing determines the incomplete specification of the microstates of systems in the Gibbs ensemble. We shall make this more precise later. First, let us examine the question as to which of the two averages (time or phase, over the Gibbs ensemble) is the primary one.

It would appear that this has an obvious answer: the primary average is the average over time or volume because it is precisely this average that is performed in physical and numerical experiments.

The opposite point of view is, however, widely used and has been very clearly formulated in the Appendix to the book by Balescu[15]: "We thus completely join the group of physicists (including, among others, Tolman and Landau) holding that the ergodic theorem is an interesting property of dynamic systems, but is irrelevant as a foundation of statistical mechanics. The way out of the difficulties mentioned above is to consider the ensemble average as the primary definition of a macroscopic dynamic function, not to be related to any other concept considered as more fundamental. The ergodic theorem is thus sidestepped. Moreover, the main difficulty mentioned above no longer subsists. The macroscopic quantity can now be a function of time."

Smoothing over the measurement time T_{meas} or over the corresponding volume V_{meas} is thus adopted as the primary average. How then can we determine phase averages in the statistical theory of nonequilibrium processes? The answer is that this can be done by constructing the Gibbs ensemble for which the degree of incompleteness corresponds to the experimental conditions. How can this be done? The answer is that the measurement parameters $T_{\text{meas}}, V_{\text{meas}}$ do not appear in the equations of the kinetic theory or the other equations in the above hierarchy of equations for macroscopic functions. However, we saw in Section 8 that the concepts of infinitesimal time interval τ_b and the corresponding volume V_b are used in the derivation of the kinetic equations. This arbitrariness in the behavior of the particles within τ_b, V_b is in fact responsible for the minimum indeterminacy in the specification of states in the Gibbs ensemble.

Let us now suppose that τ_b, V_b, and N_b have been specified, e.g., for a Boltzmann gas they are given by (9.1). This enables us to perform the smoothing of the dynamic distribution (6)

$$\tilde{f} = \overline{f^{(d)}}^{(\tau_b)} \quad \text{or} \quad \tilde{f} = \overline{f^{(d)}}^{(V_b)}. \tag{10.7}$$

Naturally, for macroscopic systems, the smoothed distributions $\tilde{f}$ are random functions, so that further averaging over the Gibbs ensemble is possible. As a result, we arrive at the statistical distribution

$$f(X,t) = \overline{\tilde{f}}(X,t) \equiv \langle \tilde{f}(X,t) \rangle. \tag{10.8}$$

In ordinary kinetic theory, it is usually implicitly assumed (because of the condition $N_b \gg 1$) that the kinetic fluctuations are negligible. The averaging of the smooth distributions $\tilde{f}$ over the Gibbs ensemble does not then lead to appreciable changes, and we have

$$f(X,t) = \overline{\tilde{f}} \approx \tilde{f} = \overline{f^{(d)}}^{(\tau_b)} \quad (\text{or} \quad \overline{f^{(d)}}^{(V_b)}), \tag{10.9}$$

which actually expresses the condition of *local ergodicity*.

When the measurement parameters $T_{\text{meas}}, V_{\text{meas}}$ and the quantities τ_b, V_b are consistently chosen, we have the approximate results

$$\overline{f}^{(T_{\text{meas}})} \approx \overline{f}^{(\tau_b)}, \quad \overline{f}^{(V_{\text{meas}})} \approx \overline{f}^{(V_b)}. \tag{10.10}$$

We now return to the criteria for the relative degree of order in nonequilibrium states of open systems. We shall make use of the results presented in the last two Sections.

11. SELF-ORGANIZATION PROCESSES IN THE VAN DER POL OSCILLATOR

It is natural to suppose that the self-organization process will take place as the feedback parameter a_p increases, i.e., as generation develops. Let us try to confirm this proposition, using a criterion based on the S-theorem.

We take a_p as the control parameter and define the stationary distribution for arbitrary a by (5.2). For the sake of convenience, we consider two characteristic states.

1. Generation threshold ($a = a_p - \gamma = 0$). We shall take this as the state of physical chaos. The corresponding distribution follows from (5.2) and is

$$f_0(E) = \left(\frac{2b}{\pi D}\right)^{1/2} \exp\left(-\frac{bE^2}{2D}\right). \tag{11.1}$$

2. Developed generation ($\varepsilon = Db/a^2 \ll 1$). From (5.2) we have

$$f(E) = \left(\frac{b}{2\pi D}\right)^{1/2} \exp\left\{-\frac{[E - (a/b)]^2}{2D/b}\right\}. \tag{11.2}$$

We can now find the entropies for the distributions (1) and (2). Calculations show that $S > S_0$, but this does not signify that the state of developed generation is more chaotic than at the generation threshold, since the effective mean energies in these states are not equal: $\langle E \rangle > \langle E \rangle_0$.

We shall now renormalize, subject to the condition that the effective Hamiltonian $H = (1/2)E^2$ remains constant. This expression follows from (1). The renormalized noise intensity in (1) can be found from an equation analogous to (5.5):

$$\tilde{D} = \frac{a^2}{b} \gg D \quad \text{for} \quad \varepsilon = \frac{Db}{a^2} \ll 1. \tag{11.3}$$

If we substitute $D \to \tilde{D}$ in (1), we find that the corresponding entropy difference is

$$\tilde{S}_0 - S = \frac{1}{2} \ln \frac{a^2}{2Db} > 0,$$

since

$$\frac{Db}{a^2} \ll 1$$
$$\frac{d(\tilde{S}_0 - S)}{da} > 0. \tag{11.4}$$

It is clear from (3) and (4) that the conditions of the S-theorem are satisfied [see (6.7) and (6.6)]. Hence we may conclude that the self-organization process takes place during the development of generation. The conclusion is almost obvious for this particular simple example. However, the situation is not so simple for more complicated oscillators (see below).

Let us compare the above result with the corresponding result based on the S-information criterion introduced by Haken.[52,53] The letter S is introduced to emphasize the contributions of Shannon to the theory of information. For the above two special cases (generation threshold and developed generation), the difference between the values of Shannon information is given by [compare with (4)]

$$I - I_0 = \ln 2 > 0. \tag{11.5}$$

We thus see that information increases by ln 2 as we proceed to the state of developed generation. This is explained by the fact that, at the generation threshold, only one half of the distribution (1) is operative, since $E > 0$, whereas both halves operate in the state of developed generation. This increase in information does not however depend on the control parameter a_p [compare with (4)] and cannot therefore be used as a characteristic of the self-organization process.

12. MORE COMPLICATED OSCILLATORS

12.1. Oscillator with inertial nonlinearity

The various "simple" dynamic systems with complex behavior[9-28,54] that have been examined include the modified (as compared with the Teodorchik oscillator) oscillator with inertial nonlinearity, which was investigated in detail by Anishchenko *et al.*[17,55] Radiophysical and numerical experiments were used by them to show that, as the feedback parameter increased (within as certain range of values of the inertial parameter), a sequence of period-doubling bifurcations occurred in the oscillator. A region of complex "chaotic" behavior was found to begin after the Feigenbaum critical point.

The S-theorem criterion was used in Ref. 56 to carry out a numerical calculation of the relative degree of order in the period-doubling region up to the Feigenbaum critical point. Renormalization was carried out for given oscillation intensity. The results of these calculations showed that, during period-doubling, i.e., as the boundary of the region of chaotic behavior (Feigenbaum critical point) was approached, the degree of order became higher, and consequently, the process of self-organization did occur according to this criterion.

An additional way of optimizing the search for the most ordered states is available for systems with two or more control parameters. Two examples of systems with two control parameters are discussed in Ref. 57.

12.2. The Van der Pol oscillator with soft and hard excitation

To extend the possibilities of control, let us examine instead of (10.2)–(10.4) an oscillator with a more complicated nonlinearity:

$$-a + bE \to -a - bE + cE^2,$$
$$a = a_p - \gamma, \quad b = b_p - \beta, \quad \gamma, \beta, c > 0. \tag{12.1}$$

where we have introduced the two feedback (pump) parameters a_p, b_p that correspond to the soft and hard excitation of generation, respectively. Our calculations have shown that for feedback parameters in the range

$$0 \leqslant a_p \leqslant a_{\max}, \; 0 \leqslant b_p \leqslant b_{\max}$$

the renormalized entropy $\tilde{S}(a_p, b_p)$ can be lower than for an oscillator with soft and hard excitation separately. A higher degree of order can thus be achieved by using two control parameters.

12.3. Van der Pol oscillator with resonant external excitation

The stationary (after averaging over the period) distribution of energy and phase can be written in the form [compare with (2.4) and (5.19) of Chapter 12 in Ref. 34]

$$f(E, \varphi) = C \exp\left\{ -\frac{(1/2b)[E - (a/b)]^2 + \sqrt{2}\, EF \cos\varphi}{D} \right\},$$
$$\int_0^\infty \int_0^{2\pi} f \, dE \frac{d\varphi}{2\pi} = 1 \tag{12.2}$$

where F is the amplitude of the external force, φ is the phase of the oscillations, and a/b is the energy of the limit cycle for $F = 0$, $D = 0$. When $F = 0$, the phase distribution is uniform, and the energy distribution is identical with (5.2).

The amplitude F and the feedback parameter a_p are now the control parameters. In the case of developed generation, the degree of order increases with increasing F because of the change in the phase distribution (it becomes nonuniform).

13. BIFURCATION OF THE ENERGY OF THE LIMIT CYCLE AND THE OSCILLATION PERIOD IN GENERALIZED VAN DER POL OSCILLATORS

We now return to (10.4) and introduce the dimensionless variables

$$t' = \omega_0 t, \quad a' = \frac{a}{\omega_0}, \quad E' = \frac{bE}{\omega_0}, \quad D' = \frac{Db}{\omega_0^2}. \tag{13.1}$$

In discrete time, $t' = \Delta n$ $(0 \leqslant \Delta \leqslant 1)$, $n = 0, 1, \ldots$, and if we take a unit step $\Delta = 1$, we obtain from (10.4) the logistic equation

$$E_{n+1} = (a+1)E_n - E_n^2 \equiv F(E_n), \quad E_{n+k} = F^{(k)}(E_n),$$
$$0 \leqslant a + 1 \leqslant L, \quad 0 \leqslant E \leqslant 4, \tag{13.2}$$

which (in different forms) is widely used both in physics and, for example, in ecology.[18,19] In the oscillator with inertial nonlinearity, it models the transition to dynamic chaos.

The logistic equation can also be used to construct mathematical models of generalized Van der Pol oscillators with two types of bifurcation stage: branching of the energy

of the limit cycle (oscillators with multistable stationary states) and period bifurcations (as well as combinations of the two types of bifurcation).[59,60] In the theory of excitable systems (see Section 15), the logistic equation can be used as a basis for a generaliation of the well-known Kolmogorov-Petrovskiĭ-Piskunov equation.[61]

Starting with (2), we obtain a sequence ($k = 1,2,3 \ldots$) of differential equations for the oscillation energy

$$\frac{dE}{dt} = \frac{1}{k}\left(F^{(k)}(E) - E\right) \quad (k = 1, 2, \ldots); \tag{13.3}$$

where we have used the correspondence rule

$$\frac{E_{n+k} - E_n}{k} \leftrightarrow \frac{dE}{dt}. \tag{13.4}$$

When $k = 1$, (3) leads to (10.4). When $k = 2$ we obtain

$$\frac{dE}{dt} = \frac{1}{2}(a - E)\,E\,[E^2 - (a + 2)\,E + a + 2]. \tag{13.5}$$

which has four stationary solutions with energy

$$\begin{gathered} E_1 = 0 \quad \text{for} \quad a \leqslant 0, \quad E_2 = a \quad \text{for} \quad 0 \leqslant a \leqslant 2, \\ E_{3,4} = \frac{a+2}{2} \pm \left[\left(\frac{a+2}{2}\right)^2 - (a+2)\right]^{1/2} \quad \text{for} \quad a \geqslant 2. \end{gathered} \tag{13.6}$$

Thus, the energy of the limit cycle is found to branch for $a = 2$, and a bistable state appears. For values of a up to the Feigenbaum critical point, the number of stationary states for given k is 2^k. The possible values of the energy of stationary states are equal to the value of E at the fixed points of (2). Equations (10.2) can be generalized in a similar way.

Let us now return to (2.2). The first of these two equations is the logistic equation, and the second follows from it after $k - 1$ iterations. If we substitute $E_{n+k} \to E_{n+1}$ in the second equation, we obtain the following set of equations:

$$E_{n+1} = F^{(k)}(E_n) \quad (k = 1, 2, \ldots). \tag{13.7}$$

When $k = 1$, this leads to the logistic equation in (2). However, when $k > 1$, equation (7) is not the same as the second equation in (2) because the left hand side of (7) contains $E_{n+1} \to E_{n+k}$. We shall show that the logistic equation generalized in this way describes new states of generation.

Figure 1(a) shows the bifurcation diagram for the logistic equation [equation (7)] with $k = 1$. The sequence of period-doubling bifurcations begins at $a = 2$. The value $a = \sqrt{8}$ corresponds to the widest window of order in the post-critical region. For $a = 3$, we have the state of most highly developed "dynamic chaos." Numerical solution of the logistic equation can be used to find the energy distribution functions. An analytic solution of (2) is possible for $a = 3$. As a result, we arrive at the Ulam-Neumann distribution

$$f(E) = \frac{1}{\pi\,[E\,(4 - E)]^{1/2}}, \quad \int_0^4 f(E)\,dE = 1. \tag{13.8}$$

A branching of the energy of the limit cycle rather than a period doubling occurs for (7) with $k = 2$ at the point $a = 2$, i.e., depending on the initial conditions, we have a bistability and the system falls either on the upper or on the lower branch (Figs. 1b and c). The period-doubling process now begins only at the point $a = \sqrt{6}$, whereas the second doubling already occurs for the logistic equation. When $a = 2.6785$ we have a chaos-chaos phase transition which gives rise to chaotic motion typical for the logistic equation (2) [(7) for $k = 1$]. This can be verified by superimposing Figs. 1b and c. We shall now consider the case $k = 3$.

For the differential equation given by (3), the limit cycle with $E = a$ is now stable up to $a = \sqrt{8}$, at which point three stationary states with different energies are found to arise.

Let us compare the bifurcation diagrams for equation (7) with $k = 1$ and $k = 3$ (Figs. 2a and b[1]). There is a clear difference between states in the widest windows of order, i.e., regions in which oscillations with period 3 are possible: Fig. 2a shows all three possible states; in Fig. 2b, only one of the three has a region of attraction that is sufficient for observation.

To determine the extent to which this difference is established by the different criteria of the relative degree of order, consider Fig. 2 which shows (for $k = 1$ and $k = 3$) the

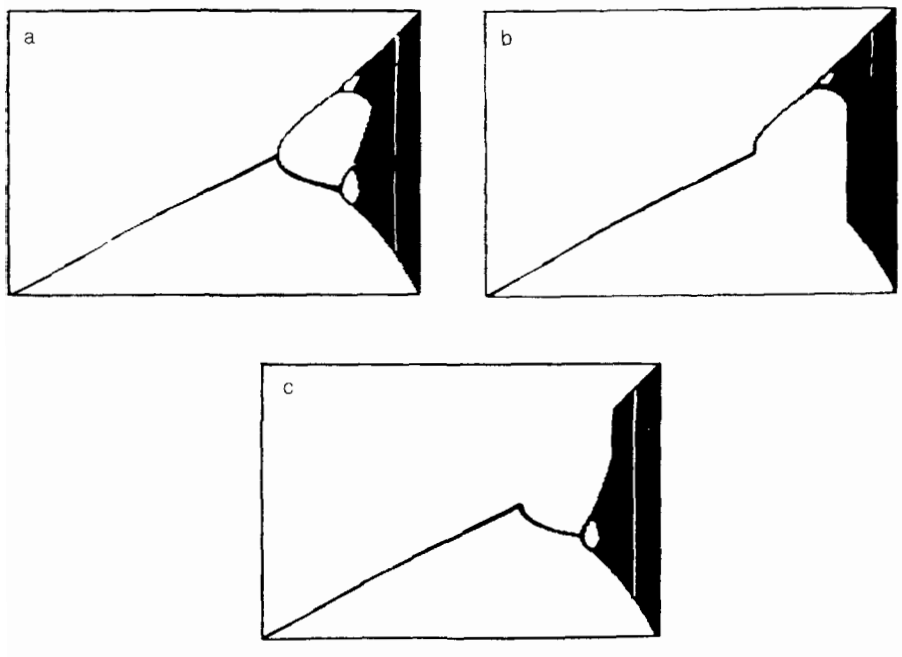

FIG. 1. Comparison of bifurcation diagrams for the logistic equation (13.7) for $k = 1(a)$ and $2(b,c)$. $a = 0 - 3.0$, $E = 0 - 4.0$. $D = 1$, $N = 10{,}000$.

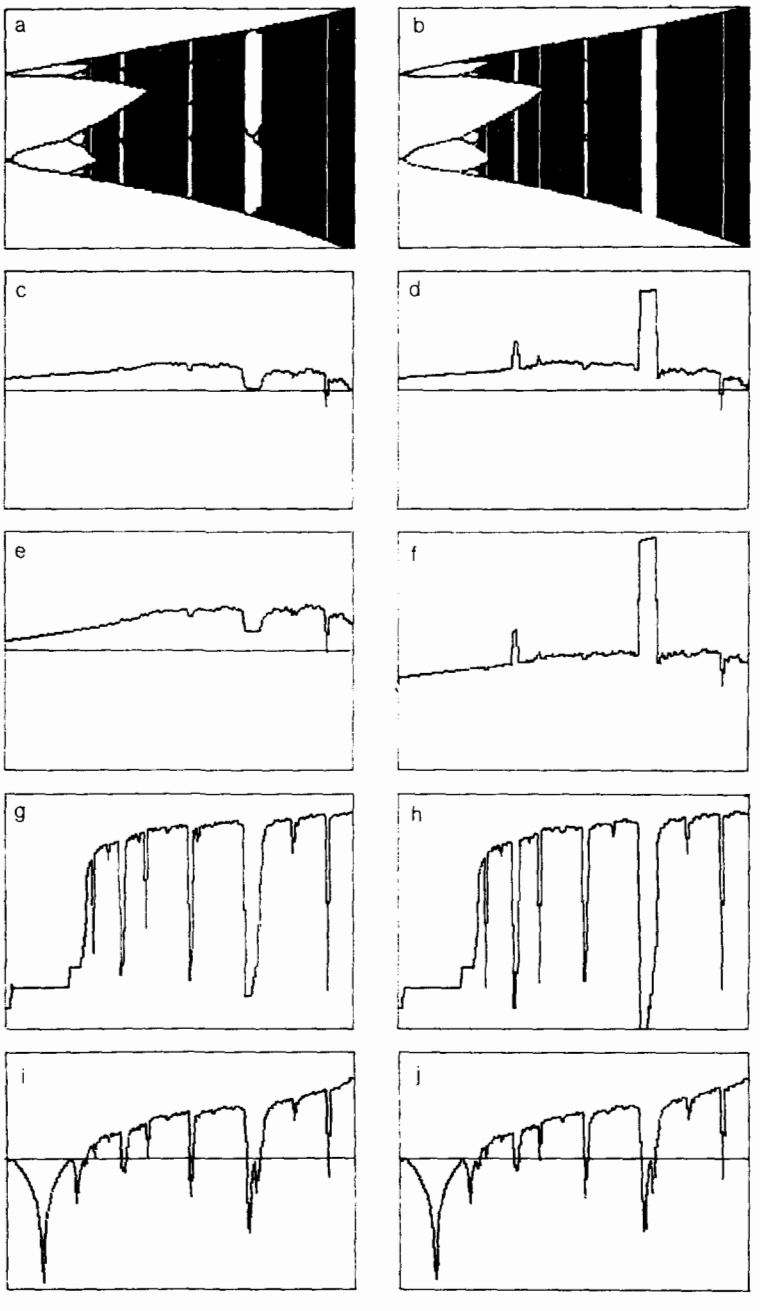

FIG. 2. Comparison of different characteristics of logistic solutions of (13.7) for $k = 1$ and 3. a,b-bifurcation diagrams, c,d-average values of energy $\langle E \rangle$, e,f-average values of the square of the energy $\langle E^2 \rangle$, g,h-average values of entropy S, i,j-average values of the Lyapunov indices as functions of the control parameter a.

dependence on a of the following quantities: the mean energy $\langle E \rangle$ (Figs. 2c and d), the mean square energy $\langle E^2 \rangle$ (Figs. 2e and f), the entropy S (Figs. 2g and h), and the Lyapunov indices found from (8.2) but now for equation (7) with $k = 1$ and $k = 3$ (Figs. 2i and j).

We see that the functions $\langle E \rangle$, $\langle E^2 \rangle$, and S exhibit more clearly the difference between states in windows of order for $k = 1$ and $k = 3$, respectively. The changes in the behavior of the Lyapunov indices are practically unnoticeable. The numerical experiment therefore exhibits the effectiveness with which the relative degree of order in nonequilibrium states can be estimated in the light of the above criteria.

14. STATISTICAL DISTRIBUTIONS FOR GENERALIZED OSCILLATORS

The Fokker-Planck equation

$$\frac{\partial f(E,t)}{\partial t} = D\frac{\partial}{\partial E}\left(E\frac{\partial f}{\partial E}\right) - \frac{\partial}{\partial E}\left[\frac{1}{k}(F^{(h)}(E) - E)f\right]. \tag{14.1}$$

corresponds to (13.3) with the Langevin source. When $k = 1$, this equation is identical with (5.1).

We now note some of the properties of the solution of (1) for $k = 2$. In this case, the corresponding dynamic equation (13.5) has a branch point for $a = 2$. Let us examine how this affects the stationary solution of (1). It will be convenient to consider three regions:

1. The region below the branch point ($a < 2$ and $Db/a^2 \ll 1$). The function $f(E)$ is then a Gaussian with variance proportional to $2/(2-a)$. Hence it follows that, as we approach the branch point, the variance increases in accordance with a kind of "Curie Law."

2. The branch point is the critical point ($a = 2$). The distribution is

$$f(E) = \frac{1}{\Gamma(1/4)}\left(\frac{2}{D}\right)^{1/4}\exp\left[-\frac{(E-a)^4}{8D}\right], \quad a = 2. \tag{14.2}$$

Thus, for $a = 2$, the variance is proportional to $\varepsilon^{1/2}$.

3. The region above the branch point. For each branch, the distribution is close to Gaussian, but with a different mean energy. The variance is proportional to $1/(a-2)$ and, consequently, again increases in accordance with a "Curie Law" as the branch point is approached.

At the branch point, the entropy (evaluated for the Gaussian distributions) has the discontinuity

$$S_1 - S_3 = \ln 2 > 0, \quad \langle E\rangle_1 \approx \langle E\rangle_2 = 2. \tag{14.3}$$

Thus, according to the S-theorem, the degree of order increases as we cross the branch point (in the direction of developing generation and increasing a). The crossing of the branch point can be looked upon as an example of a nonequilibrium phase transition. The difference between the mean energies on upper (a) and lower (b) branches now plays the role of the order parameter:

$$\eta = \langle E\rangle_a - \langle E\rangle_b = 2(a-2)^{1/2}, \quad a > a_{\text{crit}} = 2. \tag{14.4}$$

At the branch point, i.e., the critical point, we have $a = 2$ and the order parameter is zero.

15. MEDIUM CONSISTING OF COUPLED OSCILLATORS

The basic model of the theory of self-organization, or synergetics, consists of Van der Pol oscillators alongside other more complex oscillators acting as the elements of active (excitable) media. The first mathematical models of active media were proposed about 40 years ago in the well-known papers of N. Wiener, A. Rosenblut, I. M. Gel'fand, and M. L. Tsetlin. Subsequent work is reviewed in Refs. 1–4, 17, 21, 25, 28, 50, and 62–64.

At present, mathematical modeling in the theory of self-organization, i.e., synergetics, is based on reaction-diffusion equations. Specific examples of such equations have been proposed and analyzed by Kolmogorov, Petrovskiĭ, and Piskunov,[61] Zel'dovich,[65] Frank-Kamenetskii,[66] and Turing.[67] The Ginzburg-Landau equation, whose different modifications are widely used in the theory of nonequilibrium phase transitions (see, for example, Ref. 68), belongs to this class of equations.

The reaction-diffusion equations describe a class of physical, chemical, and biological phenomena. Since most of the examples constructed above were based on the model involving the Van der Pol oscillator with a symmetrized nonlinearity, we shall follow this tradition when we consider examples of distributed systems.

We begin with a simple example of diffusion of independent oscillators (Brownian particles) in space. If we confine our attention to information about the energy of the oscillators [see equation (10.4)], we arrive at the following example of the Kolmogorov-Petrovskiĭ-Piskunov (KPP) equation for the distributed energy:

$$\frac{\partial E(R,t)}{\partial t} = (a - bE)E + \mathscr{D}\frac{\partial^2 E}{\partial R^2}, \quad E(t) = \int E(R,t)\frac{dR}{V}. \tag{15.1}$$

However, in addition to spatial diffusion with diffusion coefficient $\mathscr{D}$, there is, of course, another factor that invalidates the dynamic equations (10.2)–(10.4), namely, the effect of noise on the internal degrees of freedom of an oscillator. For a given noise intensity D, the Fokker-Planck equation (5.1) for the energy distribution $f(E,t)$ corresponds to the dynamic equation for the energy of the oscillator (10.4). Both diffusion processes may play a significant role. Their combined influence can be taken into account, for example, via the Fokker-Planck equation for the general distribution $f(E,r,t)$

$$\frac{\partial f}{\partial t} = D\frac{\partial}{\partial E}\left(E\frac{\partial f}{\partial E}\right) + \frac{\partial}{\partial E}[(-a+bE)Ef] + \mathscr{D}\frac{\partial^2 f}{\partial R^2},$$
$$\frac{1}{V}\int_0^\infty dE\int dR\, f = 1. \tag{15.2}$$

The transition to equation (1) occurs for the special case

$$f(E,R,t) = \delta(E - E(R,t)), \tag{15.3}$$

which is possible when $D = 0$. On the other hand, for times much greater than the spatial diffusion time, the distribution $f(E,R,t)$ becomes spatially homogeneous, and (2) becomes identical with (1).

The most complete description of the system of oscillators, regarded as a set of elementary objects, can be based on the equation for the "N-particle distribution"

$$f_N(x_1, v_1, R_1, V_1, \ldots, x_N, v_N, R_N, V_N, t). \tag{15.4}$$

The variables x_i, v_i characterize the internal motion of the oscillators and R_i, V_i the motion of the system as a whole. The equation for the function (4) leads to (1) and (2) for the more special distributions.

Let us consider a very simple model to describe coherent processes in a system of N oscillators. We shall assume that the oscillators interact via the total energy (they have a common feedback source). Instead of (10.4), the set of dynamic equations for the functions x_i, v_i then leads to the following equation for the total energy of oscillations in the set of oscillators:

$$\frac{d\mathscr{E}}{dt} = (Na_{\text{H}} - \gamma - b\mathscr{E})\mathscr{E}, \quad \mathscr{E} = \frac{1}{2}\sum_{1\leqslant i\leqslant N}(v_i^2 + \omega_0^2 x_i^2). \tag{15.5}$$

If the noise sources in the individual oscillators are independent, the distribution $f(\mathscr{E},R,t)$ can be found with the aid of the following equation ($\mathscr{E}$ is the total energy)

$$\frac{\partial f}{\partial t} = ND\frac{\partial}{\partial \mathscr{E}}\left(\mathscr{E}\frac{\partial f}{\partial \mathscr{E}}\right) + \frac{\partial}{\partial \mathscr{E}}[(-Na_{\text{H}} + \gamma + b\mathscr{E})\mathscr{E}f] + \mathscr{D}\frac{\partial^2 f}{\partial R^2}. \tag{15.6}$$

Let us compare the stationary solutions of (2) and (6) for spatially uniform distributions of oscillators. The solution of (2) is then identical with (5.2). In special cases (at the generation threshold and under the conditions of developed generation), it assumes the form given by (11.1) and (11.2). For (6), the stationary solution can be written in the form

$$f_0(\mathscr{E}) = \exp\frac{F-H}{ND}, \quad H = (-Na_{\text{H}} + \gamma)\mathscr{E} + \frac{b}{2}\mathscr{E}^2. \tag{15.7}$$

The generation threshold $a_p = \gamma/N$ is reduced by a factor of N as compared with (11.1). When $a_p = 0$ and $b = 0$, i.e., for an ideal gas of oscillators, it follows from (7) that

$$f_0(\mathscr{E}) = \frac{ND}{\gamma}\exp\left(-\frac{\gamma\mathscr{E}}{ND}\right), \quad \langle\mathscr{E}\rangle = N\frac{D}{\gamma}. \tag{15.8}$$

Under the conditions of developed generation, for which $Db/Na_{\text{H}}^2 \ll 1$, the stationary distribution (7) assumes the form

$$f_0=\left(\frac{b}{2\pi ND}\right)^{1/2}\exp\left\{-\frac{[\mathscr{E}-(Na_{\rm H}/b)]^2}{2ND/b}\right\},$$

$$\frac{\langle(\delta\mathscr{E})^2\rangle}{\langle\mathscr{E}\rangle^2}=\frac{Db}{Na_{\rm H}^2}\propto\frac{1}{N}. \tag{15.9}$$

Thus, the effect of the collective is to reduce the relative variance by a factor of N. The increase in the degree of order can be estimated numerically on the basis of the S-theorem. To do this, we find the entropy per oscillator for the distributions given by (11.2) and (9):

$$S^{(1)}=\ln\left(\frac{2\pi D}{b}\right)^{1/2}+\frac{1}{2},$$
$$S^{(N)}=\ln\left(\frac{2\pi D}{Nb}\right)^{1/2}+\frac{1}{2}. \tag{15.10}$$

Since the corresponding average energies are equal, the entropy difference (10) determines the change in the degree of order when an oscillator is introduced into the medium of N *identical oscillators*

$$S^{(1)}-S^{(N)}=\ln N^{1/2}\geqslant 0,\quad N\geqslant 1. \tag{15.11}$$

We see that N is now the control parameter (for fixed a_p). The derivative

$$\frac{\rm d}{{\rm d}N}(S^{(1)}-S^{(N)})>0,\quad N\gg 1, \tag{15.12}$$

is then positive. The inequalities given by (11) and (12) show that $(S^{(1)}-S^{(N)})$ is now a Lyapunov function. Since inequalities (15.11) and (15.12) have the same signs, the state with $N=1$ in the "space" of the control parameter N is unstable, and the self-organization process occurs as N increases.

The Lyapunov functions Λ_F, Λ_s can also be constructed on the basis of equations (2) and (6). For example, if f_0 is a stationary solution of (2), the Lyapunov function is such that

$$\Lambda_F=D\int\ln\frac{f}{f_0}\cdot f\,{\rm d}E\,\frac{{\rm d}R}{V}\geqslant 0,\quad \frac{{\rm d}\,(F(t)-F_0)}{{\rm d}t}\leqslant 0. \tag{15.13}$$

This shows that the stationary state (for fixed $a,b,\mathscr{D},D$) is stable during temporal evolution.

We now return to the comparison of criteria for the degree of order.

16. *K*-ENTROPY AND SHANNON ENTROPY IN DYNAMICALLY UNSTABLE MOTION

The relationship between K-entropy and positive Lyapunov indices is determined by (8.1). For the one-dimensional discrete logistic equation, the Lyapunov index and, consequently, the K-entropy are determined by (8.3). The Lyapunov index given by (8.3) characterizes the role of deviations for zero initial deviations on the individual steps of the iteration process. This enables us to identify segments with exponential divergence of trajectories. In this sense, the index is a criterion for small deviations. In this approximation, the index λ typically vanishes at bifurcation points, which correpsonds to infinite correlation times. This is a manifestation of the limited value of the linear approximation. Details of the crossing of the bifurcation point need not then be considered.

In addition to (8.3), we can use the *nonlinear* characteristics of the dynamic divergence of motion:

$$K_{\rm nl}=\lim_{n\to\infty}\frac{1}{n}\sum_{k=1}^{n}\ln\frac{D(k)}{D(0)},\quad D(k)=|x_1(k)-x_2(k)|. \tag{16.1}$$

This expression gives the time average of the logarithm of the ratio of separation between trajectories at a current time k to the initial separation. In contrast to (8.3), the expression given by (1) preserves the dependence on the initial separation. In a numerical experiment, the quantity $D(0)$ can be held constant. We then have $D_{\min}(0)>0$, which means that the initial conditions cannot be repeated in a real experiment.

Another characteristic of the divergence of trajectories during temporal evolution can be the separation distribution function and the corresponding Shannon entropy

$$f(D,a),\quad S(a)=-\int\ln f(D)\cdot f(D)\,{\rm d}D. \tag{16.2}$$

For ordered regions, the function $f(D,a)$ is a set of individual lines. On the other hand, in strange attractor regions, the function $f(D,a)$ is continuous.

The stationary (invariant) distributions $f(D,a)$ are found from a numerical experiment, using two realizations $x_1(k,a)$, $x_2(k,a)$ that determine the realization of the separations $D(k,a)$. The scheme outlined in Section 7 can then be used with the corresponding distributions $f(D,a_0)$, $f(D,a_0+\Delta a)$ to determine the role of the changes a. This change is a control parameter if it leads to a reduction in the entropy renormalized to the given mean effective energy.

When the S-theorem is applied to systems with several degrees of freedom (for example, the Lorenz system, an oscillator with inertial nonlinearity, or chains of oscillators), we have to consider the choice of the distribution function (one-dimensional, different variables, multidimensional) for which the entropy is determined. For systems for which dynamic instability of motion is significant and, consequently, there are strange attractors, the separation distribution function $f(D,a)$ in the phase space of the system is probably the most informative of all the possible one-dimensional distributions.

In Section 2, "slow" time was among the possible control parameters that we enumerated. We shall now explore this further.

17. *K*-ENTROPY AND THE PRODUCTION OF ENTROPY

K-entropy is a dynamic characteristic. In this Section, we shall examine the corresponding statistical characteristics and establish their connection with the production of entropy.[69]

We shall use the time-averaged dynamic distribution of the coordinates of two trajectories

$$\tilde{f}^{(T)}(x_1,x_2,t)=\int_t^{t+T}\delta(x_1-x_1(t'))\,\delta(x_2-x_2(t'))\,{\rm d}t'. \tag{17.1}$$

In accordance with local ergodicity (see Section 10), we introduce the corresponding distribution of separations between trajectories at time t:

$$f(D,t)=\int\delta(D-|x_1-x_2|)\,f(x_1,x_2,t)\,{\rm d}x_1\,{\rm d}x_2;$$
$$\int f(D,t)\,{\rm d}D=1. \tag{17.2}$$

The corresponding entropy is

$$S(t) = -\int \ln f(D,t)\cdot f(D,t)\,\mathrm{d}D \text{ and } \frac{\mathrm{d}S}{\mathrm{d}t} = \int (-\ln f(D,t))\, I(D,t)\,\mathrm{d}D. \tag{17.3}$$

The latter is the equation of entropy balance. The production of entropy is determined by the collision integral $I(D,t)$ in the transport equation for the function $F(D,t)$. Since specific expressions for $I(D,t)$ are still unknown, we shall employ a coarser description.

We can use the distribution $f(D,t)$ to introduce two new characteristics, namely, the mean separation at time t and the effective volume (effective separation)

$$\bar{D}(t) = \int Df(D,t)\,\mathrm{d}D, \qquad \Delta D(t) = \frac{1}{f(\bar{D},t)}. \tag{17.4}$$

For small deviations $D - \bar{D}$ from the mean, the entropy (3) is approximately given by the Boltzmann formula

$$S(t) = \ln \Delta D(t). \tag{17.5}$$

This can be used to find the following two equivalent equations:

$$S(t) - S(t_0) = \ln \frac{\Delta D(t)}{\Delta D(t_0)}, \qquad \Delta D(t) = \Delta D(t_0)\exp(S(t) - S(t_0)). \tag{17.6}$$

We thus see that, with increasing entropy, which characterizes the uncertainty with which the separation between the trajectories is specified, there is an increase in the effective separation $\Delta D(t)$. The mean rate of change of entropy within the time interval $t - t_0$, i.e., the statistical analog of K-entropy, can now be defined with the aid of (6):

$$K_{\text{stat}} = \frac{S(t) - S(t_0)}{t - t_0} = \frac{1}{t - t_0}\ln\frac{\Delta D(t)}{\Delta D(t_0)}. \tag{17.7}$$

Hence, it follows that K_{stat} determines the entropy production averaged over a finite interval. Local changes are defined by the corresponding equation of entropy balance that follows from (5) and takes the form

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\ln \Delta D(t) \equiv \sigma(t). \tag{17.8}$$

We see that the production of entropy has a constant sign: it increases if the effective separation between trajectories increases with time, and decreases otherwise.

18. EVOLUTION OF ENTROPY IN A TRANSITION FROM LAMINAR TO TURBULENT FLOW

"I recall that von Karman said in his introduction that, when he finally faces the Creator, his first supplication will be to ask for the revelation of the secret of turbulence." (H. Moffatt)

Of the numerous questions that arise in the theory of turbulence, we consider only one: is the transition from laminar to stationary turbulent flow a transition from a more ordered to a less ordered state or not?

The immediate answer that comes to mind is that the transition from laminar to turbulent flow is a transition to a *more chaotic state*. This is clearly expressed, for example, on p. 9 of Ref. 70: "Turbulent motion is chaotic. The term 'chaotic' is in this case almost synonomous with 'turbulent.' "

However, the opposite view has also been expressed (see Chapter 24 in Ref. 34). It is represented by the following statement in Ref. 58: "Turbulence has for long been identified with chaos or noise. We now know that this is not so ... . The transition from laminar to turbulent flow is a self-organization process. Part of the energy of the system which, in the case of laminar flow, is taken up by the thermal motion of the molecules, is transformed into organized macroscopic motion." This picture can be looked upon as a verbal description of the theory developed in Ref. 40 (see also Refs. 41 and 38), which we shall now summarize.

We take the state of local equilibrium in laminar flow as the state of physical chaos. It is characterized by the distribution

$$f_l(r,v) = \left(\frac{m}{2\pi kT}\right)^{3/2}\exp\left[-\frac{m(v - u_l(r))^2}{2kT}\right], \tag{18.1}$$

where $u_l(r)$ is the velocity of the laminar flow at the point r. The entropy is

$$S_l(r) = -nk\int \ln f_l(r,v)\cdot f_l(r,v)\,\mathrm{d}v, \quad n = \frac{N}{\hat{V}}. \tag{18.2}$$

In turbulent flow, the hydrodynamic velocity is a random function, so that the following distribution is also random:

$$\tilde{f}_t(r,v,t) = \left(\frac{m}{2\pi kT}\right)^{3/2}\exp\left[-\frac{m(v - \tilde{u}(r,t))^2}{2kT}\right]. \tag{18.3}$$

The average entropy

$$S_t = \langle \tilde{S}_t\rangle = -nk\int \langle \ln \tilde{f}_t\cdot\tilde{f}_t\rangle\,\mathrm{d}v \tag{18.4}$$

can serve as a measure of uncertainty. The effective Hamiltonian is determined by the structure of the distribution (1), so that the additional condition (5.5) now takes the form

$$\int \frac{m}{2}(v - u_l)^2 f_l\,\mathrm{d}v = \int \frac{m}{2}(v - u_t)^2\bar{\tilde{f}}\,\mathrm{d}v \tag{18.5}$$

where $u_t = \langle \tilde{u}\rangle$ is the average turbulent velocity.

The additional condition given by (5) can be compared with the condition $(1/2)\langle E^2\rangle = \text{const}$ for the Van der Pol oscillator. The expression given by (11.3) follows from it. The additional chaotic motion introduced in this way at the generation threshold in the case of fully developed generation becomes more organized.

The additional condition (5) leads to an analogous consequence. It follows from it that, according to the criterion provided by the S-theorem, the comparison is performed at different temperatures $T_l, T_t \equiv T$ such that

$$kT_t = kT + \frac{1}{3}m\langle(\delta u)^2\rangle > kT, \tag{18.6}$$

where δu are fluctuations in the hydrodynamic velocity. The temperature difference is thus determined by the Reynolds stress. Using (6), we find that the required expression for the entropy difference is

$$T(S_l - S_t) = \frac{3}{2}kTn\ln\frac{kT + (m/3)\langle(\delta u)^2\rangle}{kT} \approx \frac{mn}{2}\langle(\delta u)^2\rangle. \tag{18.7}$$

The corresponding derivative with respect to the control parameter is

$$\frac{\mathrm{d}}{\mathrm{d}\,\mathrm{Re}}(S_l - S_t) > 0. \tag{18.8}$$

The results given by (18.7) and (18.8) show that the entropy difference $S_l - S_t$ is a Lyapunov function and that the

laminar flow adopted as the state of physical chaos is unstable. This leads us to the conclusion that the transition from laminar to stationary turbulent flow is an example of a self-organization process.

The greater ordering of the turbulent flow is manifested in, among other things, the appearance of turbulent viscosity. Momentum transfer from layer to layer in the hydrodynamic flow then occurs not at the molecular level, as in laminar flow, but is now a cooperative phenomenon.

In other words: the individual, unorganized resistance in the case of laminar flow is replaced in the transition with collective, and therefore more organized, resistance.

The relative degree of order in hydrodynamic flow and oscillators, deduced from the criterion provided by the S-theorem, is also discussed in Refs. 73 and 74.

We have thus shown, using the S-theorem formulated for evolution processes in the space of control parameters, *that stationary turbulent flow can be more ordered, i.e.,* more highly organized, than laminar flow. Of course, the greater degree of order in turbulent motion can also be demonstrated by considering the temporal evolution of a closed system from the initial nonequilibrium motion to the final equilibrium motion. The H-theorem then shows that this is accompanied by an increase in entropy and, consequently, the process of evolution gives rise not to self-organization, but to the degradation of the initially more ordered state (see the end of Section 2). The presence of degradation is indicated by an increase in temperature. Consider a simple example.

Suppose that homogeneous turbulence with the distribution given by (18.3) is created in a closed system at the initial time. The process of evolution then establishes the equilibrium state with the distribution f_0 given by (18.1) for $u_l = 0$ and entropy S_0. Since the system is macroscopic, the energy will be practically equal to its mean value, so that the relative degree of order of the initial (turbulent) and equilibrium motions can be characterized by the entropy difference $\langle \tilde{S}_t \rangle, S_0$. If the velocity $\tilde{u}$ is small in comparison with the thermal velocity, the deviations $\delta\tilde{f} = \tilde{f} - f_0$ are small and the entropy difference is given by

$$S_0 - \langle \tilde{S}_t \rangle = \frac{kn}{2} \int \frac{\langle \delta\tilde{f}\delta\tilde{f} \rangle}{f_0} \, dv = \frac{kn}{2} \int \left(\frac{m\tilde{v}\tilde{u}}{kT} \right)^2 f_0 \, dv \geqslant 0. \quad (18.9)$$

After integration, we then again arrive at (7)!

If we repeat the experiment for different initial conditions, we can use the temperature of the equilibrium states to judge the relative degree of order in the two initial turbulent motions.

19. ENTROPY PRODUCTION IN LAMINAR AND TURBULENT FLOWS

Entropy production (alongside entropy itself) can serve as a comparative measure of the degree of order in open systems. We shall illustrate this by considering the transition from laminar to stationary turbulent flow.

Following Ref. 71, let us compare entropy production in a stationary average turbulent flow that arises for Reynolds numbers $\mathrm{Re} > (\mathrm{Re})_{\mathrm{crit}}$ and an imagined laminar flow (that is unstable for these Reynolds numbers). It is shown in Ref. 71 that, subject to the additional condition that the stresses on the channel walls are equal for these flows, i.e., the dynamic velocities v_* are equal, the entropy production is less for the turbulent flow (σ_t) than for the laminar flow (which is unstable under these conditions), i.e., $\sigma_t < \sigma_l$.

The actual process thus proceeds along the path with the lower entropy production. This can be taken to be an indication of a higher degree of order in the turbulent flow, and the transition from laminar to average turbulent flow can be regarded as a self-organization process.

As an illustration, we reproduce the result obtained by calculating entropy production for Couette flow in a plane channel[71]:

$$\frac{\sigma_t}{\sigma_l} = \frac{\mathrm{Re}}{2\mathrm{R}_*^2} \leqslant 1 \quad (19.1)$$

in which the characteristic Reynolds numbers are given by

$$\mathrm{Re} = \frac{2uh}{\nu}, \quad \mathrm{R}_* = \frac{v_* h}{\nu}, \quad (19.2)$$

v_* is dynamic velocity, h is the separation between the planes, and $2u$ is the relative velocity of the planes. The equals sign refers to laminar flow in which the law of resistance takes the form $\mathrm{Re} = 2\mathrm{R}_*^2$. For the turbulent flow, this means that ratio σ_t/σ_l is less than unity. For developed turbulence

$$\frac{\sigma_{\text{т}}}{\sigma_{\text{л}}} = \frac{1}{\varkappa} \frac{\ln \mathrm{Re}}{\mathrm{Re}} < 1, \quad \mathrm{Re} \gg (\mathrm{Re})_{\mathrm{crit}}. \quad (19.3)$$

where $\varkappa = 0{,}4$ is the von Karman constant.

The turbulent and laminar entropy production was calculated in Ref. 71 under the additional assumption that the stresses on the walls were constant. The choice of this condition was dictated by the structure of the expression for the entropy production and the form of the law of resistance.

We can now use the above special case as a basis for formulating the principle of self-organization in terms of the entropy production criterion.

20. THE PRINCIPLE OF MINIMUM ENTROPY PRODUCTION IN SELF-ORGANIZATION

Prigogine (see Refs. 36 and 72) has formulated the principle of minimum entropy produciton in stationary states. The essence of this is as folllows:

$$\sigma(t) \geqslant \sigma_{\mathrm{st}}, \quad (20.1)$$

where σ_{st} is the entropy production in the stationary state and $\sigma(t)$ is the entropy production in the current (nonstationary) state. The validity of this result has been demonstrated only for linear systems. A general proof for nonlinear systems has been lacking. On the other hand, there are known examples in which this principle is violated.[36]

Let us now return to inequality (19.1). It determines the ratio of two quantities, namely, entropy production in stable average turbulent flow and the corresponding quantity for unstable (for the same Reynolds number) laminar flow. Basing ourselves on this example, we formulate a proposition which we shall refer to as the *principle of minimum entropy production in self-organization processes*. The essence of this principle is as follows.

Consider a self-organization process consisting of a sequence of nonequilibrium phase transitions. Let a_{crit} be the critical value of the control parameter for which the successive bifurcation takes place. Let σ_{stab} represent the entropy production in the next stable state. The entropy production σ_t in turbulent flow corresponds to this quantity. The pre-

bifurcation state becomes unstable for $a > a_{crit}$. Let σ_{instab} represent the corresponding entropy production. It corresponds to σ_l for the imagined (unstable in the postcritical region) laminar flow. The calculation of σ_{instab} and σ_{stab} must again be performed under the additional condition whose specific form depends on the nature of the process under consideration. In our notation, the principle formulated above can be expressed as the inequality

$$\sigma_{instab} > \sigma_{stab}. \tag{20.2}$$

This means that, in nonequilibrium phase transitons constituting a self-organization process, the system proceeds along the path of decreasing entropy production.

A general proof of this principle remains an open question. It is reasonable to suppose, however, that the above special case will stimulate research in this area.

21. CONCLUSION

To conclude our review, let us consider a mathematical model of biological evolution that will reveal a further important function of entropy.

21.1. Entropy as a measure of diversity in biological evolution

We have seen that the Boltzmann-Gobbs-Shannon entropy can be used (in addition to its traditional role in statistical theory and the theory of information) as a measure of relative degree of order in self-organization processes. We shall now show that it can play a further part, namely, it can be a measure of the diversity that is necessary for natural selection in biological evolution. To do this, we must extend the class of mathematical models discussed in the respective papers of Eigen, Vol'kenshtein, Ebeling, and others.[30–32,75]

As before, we shall characterize the state of the system by the distribution $f(X,t)$ of a set of variables X. In addition to the entropy $S = \langle S \rangle = -\int \ln f \cdot f\, dX$, we shall consider the unaveraged, i.e., fluctuating, entropy $\ln f(X,t)$. For the uniform distribution, $f = 1/\Omega$, where Ω is the domain of the variables.

$$W(X, t) = \ln (f(X, t)\,\Omega). \tag{21.1}$$

For the uniform distribution, for which $f = 1/\Omega$, this function is zero, so that there is no diversity. According to (1) the mean diversity is given by

$$\langle W \rangle = S_0 - \langle S \rangle, \quad S_0 = \ln \Omega \tag{21.2}$$

and is therefore determined by the difference between the entropies $S_0, \langle S \rangle$.

We shall follow Ref. 75 and use the model reaction-diffusion equation [cf. (15.1)] for the distribution function $f(X,t)$. However, the reactive term will now be expressed in terms of the fluctuation of diversity. This leads to the equation

$$\frac{\partial f}{\partial t} = \alpha (\ln f - \langle \ln f \rangle) f + D \frac{\partial^2 f}{\partial X^2}, \quad \int f\, dX = 1. \tag{21.3}$$

The coefficient α will be referred to as the *evolution parameter* because the character of the process depends significantly on the sign of α. In (3), D is the intensity of noise that is responsible for mutations in the individual elements of the system under consideration

$$\frac{d\langle S \rangle}{dt} = -\frac{d\langle W \rangle}{dt} = -\alpha \langle (\ln f - \langle \ln f \rangle)^2 \rangle + D \int \frac{1}{f} \left(\frac{\partial f}{\partial X} \right)^2 dX. \tag{21.4}$$

Consider the following three special cases.

(1) $\alpha = 0$. Equation (4) now reduces to the entropy balance equation for a diffusion process. During evolution to the homogeneous distribution, the mean diversity W decreases and the entropy increases. This is an example of the H theorem.

(2) $\alpha < 0$. Both terms on the right-hand side of (4) are positive and the process proceeds to the equilibrium state: $f = 1/\Omega$, $W = \langle W \rangle = 0$.

(3) $\alpha > 0$. Fluctuations in diversity reduce the mean entropy and, consequently, increase the mean diversity. In the stationary state, the entropy balance equation assumes the form

$$\alpha \langle (\ln f - \langle \ln f \rangle)^2 \rangle \equiv \alpha \langle (W - \langle W \rangle)^2 \rangle = D \int \frac{1}{f} \left(\frac{\partial f}{\partial X} \right)^2 dX. \tag{21.5}$$

We thus reach the stationary state with zero entropy production, in which the variance of diversity is finite and is determined by the intensity of the noise that gives rise to mutations. We thus have the possibility of natural selection.

In the stationary state, equation (3) assumes the following form for $\alpha > 0$:

$$D \frac{\partial^2 f}{\partial X^2} + \alpha \ln f \cdot f = \alpha \langle \ln f \rangle f, \quad \int f\, dX = 1. \tag{21.6}$$

We thus have a peculiar eigenvalue problem in which the eigenvalue is the mean logarithm of the required distribution function, i.e., the entropy or mean diversity [cf. equation (1) in Section 10 of Ref. 76].

21.2. Some problems in the statistical theory of open systems

The above self-organization criteria were illustrated by simple examples. Of course, they can also be used to analyze self-organization processes in systems that are of greater practical importance, i.e., plasma processes,[76] optical systems,[78–79] and forecasting problems.[80] Other examples include physical, chemical, and biological systems in which the reaction-diffusion type equations are employed (in addition to those cited above; see Refs. 81 and 82).

The criteria for chaos based on fractal dimension play a major role in the theory of dynamic chaos.[17,22,26,27,83,84] The role of the fractal dimension in the statistical theory of nonequilibrium processes is interesting and requires separate discussion.

The description of chaotic motion in quantum systems has become particularly important in recent years. The relevant literature is cited in a recent review.[85] Here, we merely note that many of the results presented above can be extended to quantum systems.

In the examples discussed above, the control parameters were assumed to vary quasistatically, and entropy was expressed in terms of one-time distributions. Relaxation of these restrictions and, in particular, the use of two-time distribution functions will of course open up extensive new avenues for the theory of self-organization.

Finally, we note the book entitled *Principles of Self-organization*[86] which is a collection of papers presented at what appears to have been the first symposium on problems of

self-organization. It was held in 1961 in the Laboratory for the application of computers in biology at the Illinois University in the United States. The editor of the translation into Russian writes in his introduction "...self-organization has remained over many centuries perhaps the most puzzling phenomenon, the most intimate secret of nature... . The reader will not find a single paper in this collection that claims to reveal the principles of self-organization."

These words were written more than a quarter of a century ago. We have to ask whether during this time we have advanced in our understanding of the principles of self-organization. To some extent the answer must be in the affirmative. However, there are still many more unsolved problems than final results. This will stimulate greater interest in this new and rapidly developing interdisciplinary subject.

[1)]Figs. 2*a-j* were obtained by V. I. Chetverikov.

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