Definition of the Degree of Order in Selforganization Processes

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Abstract. Selforganization processes controlled by two pumping parameters are studied. The question of thermodynamic equilibrium in nonlinear pumped systems is investigated. Using the entropy statement formulated in a recent paper the degree of order of steady states is defined. It is shown that those systems can be optimated following various principles. For illustration, selfoscillations of nonlinear oscillators with two pumping parameters are studied.

Zur Bestimmung des Ordnungsgrades bei Selbstorganisationsprozessen

Inhaltsübersicht. Es werden Selbstorganisationsprozesse betrachtet, die durch zwei Parameter gesteuert werden. Die Lage des thermodynamischen Gleichgewichts in nichtlinearen gepumpten Systemen wird untersucht. Zur Bestimmung des Ordnungsgrades stationärer Zustände wird der in einer vorhergehenden Arbeit formulierte Entropiesatz verwendet. Es wird gezeigt, daß derartige Systeme nach verschiedenen Kriterien optimiert werden können. Als Illustration dienen selbsterregte nichtlineare Oszillatoren mit zwei Steuerparametern.

1. Introduction

The investigation of selforganization processes in many systems makes it indispensable to define the degree of order of a sequence of states corresponding to different values of the control parameters.

Of course, one can estimate the order or disorder following various criteria [1]. A recent paper [2] used the BOLTZMANN-GIBBS entropy and formulated the following statement called the S-theorem: With increasing distance from equilibrium the entropy-values of steady states renormalized to a fixed value of the "mean energy" decrease.

The S-theorem as well as the H-theorem cannot be proved in a general form. However the S-theorem can serve as an "measuring instrument" in the selforganization theory. The validity of the S-theorem was proved for VAN DER POL oscillators of the THOMSON type [2], for generators with an inertial nonlinearity [3], for generalized VAN DER POL oscillators with a sequence of limit cycles [4], for the transition from laminar to turbulent flows [5]. The latter example confirmed the point of view stated in [6] that turbulent structures are more ordered or more highly organized than laminar. This point of view has been strengthened also in [7, 8] as well as in [9] which compared the entropy production of a turbulent and a mental laminar flow in channels at fixed tension at the wall. In all of these examples selforganization processes are controlled by one parameter only: In generators it is the feedback, in flows the REYNOLDS number. In the present paper we investigate two examples in which selforganization is regulated by two control parameters.

1. We will consider a VAN DER POL oscillator with hard or weak excitation (depending on the values of the linear and the first nonlinear friction coefficients). We will choose two control parameters which can be called coefficients of linear and nonlinear feedback, respectively.

2. As the second example we will study a VAN DER POL oscillator with weak excitation influenced by a resonance force. In this case the control parameters will be the linear feedback and, for instance, the amplitude of the external force.

Naturally, in the presence of two pumping parameters selforganization processes become more complicate. A number of new questions arises, we try to answer some of them in this paper. The first question consists in the choice of the equilibrium state which serves as the origin of the level of chaos. In the following the state corresponding to zero values of the chosen control parameters will be identified with the "equilibrium". The second question is connected with finding new possibilities for the increase of the degree of order using two control parameters in comparison with a one-parameter system. As we will show, there are various approaches for solving this problem.

2. VAN DER POLS Oscillators with Two Control Parameters

2.1. Oscillator with Two Types of Feedback

Our first system may be discribed by the LANGEVIN equations

$$\begin{split} \frac{d\tilde{x}}{dt} &= \tilde{v}, \\ \frac{d\tilde{v}}{dt} &+ \left(a + \frac{2}{3}b\tilde{v}^2 + \frac{4}{5}c\tilde{v}^4\right)\tilde{v} + \omega_0^2\tilde{x} = \sqrt{D}\,y(t) + \frac{\tilde{v}}{2}\frac{\partial D}{\partial\tilde{E}}, \\ \langle y(t) \rangle &= 0, \quad \langle y(t), y(t') \rangle = 2\delta(t-t'), \\ a &= \gamma - a_p, \, b = b_0 - b_p, \, \tilde{E} = \frac{1}{2}(\omega^2\tilde{x}^2 + \tilde{v}^2), \, m = 1, \end{split}$$
(1)

 γ and b_0 are the linear and the first nonlinear friction coefficients respectively, a_p and b_p the linear and the nonlinear feedback. For mathematical simplicity we consider only GAUSSIAN white noise with energy-dependent intensity and only generators of the THOM-SON type. We introduce slow variables x, v by the transformation

$$\tilde{x} = x \cos \omega_0 t + \frac{v}{\omega_0} \sin \omega_0 t, \ \tilde{v} = v \cos \omega_0 t - \omega_0 x \sin \omega_0 t.$$

Using an averaging over the oscillation period $2\pi/\omega_0$ we get

$$\begin{aligned} \frac{dE}{dt} + (a + bE + cE^2) & E = \sqrt{D} y_E(t) + \frac{1}{2} E \frac{\partial D}{\partial E}, \\ y_E(t) &= \omega_0^2 x y_x(t) + v y_v(t), \\ y_x(t) &= -\frac{1}{\omega_0} \sin \omega_0 t \cdot y(t), \quad y_v(t) = \cos \omega_0 t \cdot y(t). \end{aligned}$$
(2)

Of course, $E = \tilde{E}$. We obtain the corresponding FOKKER-PLANCK-equation (FPE)

$$\frac{\partial}{\partial t}f(E,t) = \frac{\partial}{\partial E}\left(D \cdot E\frac{\partial}{\partial E}f\right) + \frac{\partial}{\partial E}\left[\left(a + bE + cE^2\right)Ef\right].$$
(3)

It is interesting to note that (2) and (3) are approximations for (1), however they are exact equations for the following system [4]:

$$\frac{dx}{dt} + \frac{1}{2} \left(a + bE + cE^2\right) x = v + y_x(t) \sqrt{D} + \frac{1}{4\omega_0^2} \frac{\partial}{\partial x} D,$$

$$\frac{dv}{dt} + \frac{1}{2} \left(a + bE + cE^2\right] v + \omega_0^2 x = y_v(t) \sqrt{D} + \frac{1}{4} \frac{\partial}{\partial v} D.$$
(4)

There are two types of noise intensity:

(i) The noise is given a priori, i.e. it does not depend on the deterministic characteristics of the actual system. Here we will consider additive noise only, $D = D_0 = \text{const.}$

(ii) The noise is natural [4]. Natural we will call any noise that is "synchronized" with the system in the following way: If all feedbacks vanish the natural noise should guarantee that the stationary probability distribution coincides with the equilibric BOLTZMANN-GIBBS function (5)

$$f(E) = \frac{\gamma}{D_0} \exp\left(-\frac{\gamma E}{D_0}\right), \quad D_0 = \gamma kT, \langle E \rangle = kT.$$
(5)

This means that the natural noise satisfies a generalized EINSTEIN-formula (6). Such a generalization is valid for systems with a nonlinearity of dissipative type [10]. Substituting f(E) in the stationary FPE (3) for (5) we obtain in general

$$D(E) = 2e^{2E/kT} \int_{E}^{\infty} P_0(E') e^{-2E'/kT} dE', \quad D(0) > 0.$$
(6)

In our special case $P_0(E) = \gamma + b_0 E + cE^2$.

In a linear system with $P_0 = \gamma$ one obtains the well known EINSTEIN-formula $D_0 = \gamma kT$. We emphasize that as a result of the kinetic theory we use the same FPE (3) for given noise (additive or multiplicative) as well as for natural noise. Therefore we included in the LANGEVIN equations (1) and (4) the terms with the derivatives of the noise intensity.

Let us now solve the stationary FPE (3).

(i) Considering given noise we obtain

$$f(E) = \frac{1}{Z} \exp\left[-\frac{aE + \frac{b}{2}E^2 + \frac{c}{3}E^3}{D_0}\right], \quad \int_0^\infty f(E) \, dE = 1. \tag{7}$$

There is another convenient form

$$f(E) = \exp\left[\frac{F - H(E) + U_1(E)}{D_0}\right],$$
(7*)

 $F = -D_0 \ln Z$ may be called the "effective free energy",

 $H = \gamma E + \frac{b_0}{Z} E^2 + \frac{c}{3} E^3$ the "effective Hamiltonian" because of the analogy of (7*) and the canonical GIBBS distribution.

 $U_1 = a_p E + \frac{b_p}{Z} E^2$ is a function of the pumping parameters which defines the deviation from the "canonical" distribution.

(ii) Now we consider natural noise and obtain

$$f(E) = \frac{1}{Z} e^{-E/kT} \exp\left[\int_{0}^{E} \frac{P_{p}(E')}{kT P_{0}(E')} dE'\right], \quad \int_{0}^{\infty} f(E) dE = 1.$$

In our special system is $P_0(E) = \gamma + b_0 E + cE^2$, $P_p(E) = a_p + b_p E$, $P_0(0) = \gamma > 0$, $P_0(0) - P_p(0) = \gamma - a_p > 0$,

$$f(E) = \frac{1}{Z} e^{-E/kT} [P_0(E)]^A \exp\left[\frac{a_p c - b_p b_0}{kT cB} \arctan\frac{2cE + b_0}{B}\right],$$

$$A = \frac{bp}{2ckT}, \quad B = \sqrt{4\gamma c - b_0^2}.$$
(8)

2.2. Oscillator with a Resonance Force

Our second example is given by the equations

$$\frac{d\tilde{x}}{dt} = \tilde{v},$$

$$\frac{d\tilde{v}}{dt} + \left(a + \frac{2}{3}b_0\tilde{v}^2\right)\tilde{v} + \omega_0^2\tilde{x} = \bar{X}\cos\omega_0 t + \sqrt{D}y(t) + \frac{1}{2}\tilde{v}\frac{\partial D}{\partial E},$$

$$\langle y(t) \rangle = 0, \langle y(t), y(t') \rangle = 2\delta(t - t'), \ a = \gamma - a_p.$$
(9)

We obtain the corresponding FPE (10) for (9) in the case of quasiharmonical oscillations as well as for the system with symmetric dissipation terms (in analogy to (4)).

$$\frac{\partial}{\partial t}f(x,v,t) = \frac{1}{2}\frac{\partial}{\partial x}\left[(a+b_{0}E)xf\right] + \frac{1}{2}\frac{\partial}{\partial v}\left[(a+b_{0}E)vf\right] \\ + \frac{1}{2\omega_{0}^{2}}\frac{\partial}{\partial x}\left[D\frac{\partial}{\partial x}f\right] + \frac{1}{2}\frac{\partial}{\partial v}\left[D\frac{\partial}{\partial v}f\right] - \frac{1}{2}\frac{\partial}{\partial v}\left[\bar{X}f\right].$$
⁽¹⁰⁾

It has the following stationary solution in the case of given noise

$$f(x,v) = \frac{1}{Z} \exp\left[-\frac{aE + \frac{b_0}{2}E^2 - v\bar{X}}{D_0}\right], \quad \int_{-\infty}^{\infty} f(x,v) \, dx \, dv = 1.$$
(11)

We introduce again

$$F = -D_0 \ln Z, \ H = \gamma E + \frac{b_0}{2} E^2, \ U_1 = a_p E + v \bar{X}$$
(12)

and (11) can be written again in the form (7^*) .

3. Thermodynamic Equilibrium in Nonlinear Systems

It is natural to choose as the origin of the degree of order the state of maximal chaos — the equilibrium. From thermodynamics it is well known that the equilibrium probability distribution depends essentially on the influence of the surroundings on the system. For instance, a system in a thermostat is discribed in equilibrium by the canonical GIBBS function. A BROWNIAN particle in a medium or an oscillator are examples for this situation.

In nonlinear open systems, however, the situation is more difficult. If the system is pumped by flows of energy, particles a.o., there can be nonequilibrium steady states too. Nevertheless, under certain conditions these systems also show equilibrium-like behaviour (we will speak about "equilibrium" state). Let us sum up the conditions: First, all the feedbacks have to vanish, i.e. all the pumping parameters have to go to zero, the probability distribution is the "canonical" (7*), with U = 0. "Equilibrium" means that the system will relax to the state of rest. For systems with given noise this condition can be satisfied only for definite parameter ranges. We demonstrate this on our examples (7) and (11). The system (11) is closed if $a_p = \bar{X} = 0$. The nonequilibrium steady state (a limit cycle with the energy $E_0 = -\frac{a}{b_0} = -\frac{\gamma}{b_0}$ is vanishing if $\gamma > 0$. Only for $b_0 > 0$ the distribution function can be normalized. Hence for all positive γ our system relaxes to the "equilibrium" (Figs. 1, 2). In system (7) the feedbacks vanish if $a_p = b_p = 0$. There can be two limit cycles with the energies $E_{1,2} = -\frac{1}{2c} \left[b \pm \sqrt{b^2 - 4ac} \right] = -\frac{1}{2c} \left[\frac{b_0}{c} \pm \sqrt{b_0^2 - 4\gamma c} \right]$. They vanish if $\frac{b_0}{c} > -2 \sqrt{\frac{\gamma}{c}}$, we assume $\gamma > 0$ and c > 0. Hence with all of these γ and b_0 the system (7) relaxes to the state of rest (Figs. 3, 4).





Fig. 1. Equilibrium and nonequilibrium steady states of (9) for $\overline{X} = 0$. "0" corresponds to "equilibrium"







Fig. 3. Equilibrium and nonequilibrium steady states of (1), (4)

Fig. 4. Parameter range of (1), (4), in which "equilibrium" is possible

4. The GIBBS-theorem for Open Systems and the S-theorem

Let us recall the well known GIBBS-theorem [6]. We consider two distribution functions, first the canonical GIBBS function

$$f_0(X) = \exp\left[\frac{F(a, T) - H(X, a)}{kT}\right],$$

X is a complete set of coordinates and momenta, "a" is a parameter set, H is the Hamiltonian and F the free energy. Any second distribution function can be represented in the form (7^{*}) introducing a control parameter function U_1

$$f_1(x) = \exp\left[\frac{F(a, T) - H(X, a) + U_1(X, a)}{kT}\right]$$

In the validity of two conditions, the normalization (13) and the constance of the mean energy (14)

$$\int dX f_0(X) = \int dX f_1(X) = 1,$$
(13)

$$\int dX \, H(X) \, f_0(X) = \int dX \, H(X) \, f_1(X) \equiv U_0, \tag{14}$$

the theorem states that the entropy has its maximum in the equilibrium and that $S_0 = S_1$ only for $f_1 \equiv f_0$, where the BOLTZMANN-GIBBS entropy is defined by $S = -k \int dX \ln f \cdot f$. In the case of open systems however, the mean energy does not remain on the equilibrium level. That means that the condition (14), as a rule, is not holding. On the other hand, if one wants to compare the entropy of states corresponding to different values of the control parameters, one at the same time has to fix the mean energy. This can be achieved by corresponding changes of one or several external non-pumping parameters. In recent papers this approach has been demonstrated for oscillators [2] and also for hydrodynamic flows [5, 8], where the intensity of given noise and temperature, respectively, were changed. Using this idea we can present the condition (14) in the form (14*).

$$\int dX \, H(X) \, f_0(X) = \int dX \, H(X) \, \tilde{f}_1(X) \equiv U_0, \tag{14*}$$

there is $\tilde{f}_1 \equiv f_1 \mid$, the functional $\tilde{T}[U_1(X)]$ is the solution of (14*), and we obtain the more general extrement

the more general statement

$$S_0 \ge S_1 = -k \int dX \ln f_1 \cdot f_1.$$

The proof follows exactly the classical GIBBS proof [6].

It is necessary to stress that the theorem holds for any function H, even if it is not a Hamiltonian. In systems with several control parameters the choice of the "effective HAMILTON function" is closely connected with the definition of the "equilibrium".

For open systems, however, the S-theorem makes a stronger statement, since it asserts that the entropy of nonequilibrium states decreases monotonously with increasing distance from the "equilibrium", (here and in the following we mean the entropy \tilde{S}_1). As we have mentioned the S-theorem was proved for several systems with one control parameter. However, in the case of two parameters it is not always clear how to define and to measure the distance from "equilibrium". In this situation we will "employ" the S-theorem as a "measuring instrument", we will take the entropy as a measure of the distance from "equilibrium". This approach seems to be justified since in classical statistical physics entropy is the best and most general measure of order we know. Naturally, that means that the S-theorem becomes our basic hypothesis. But in the present moment there is no reason for doubts about its general validity. Of course, for any concrete system other more specific measures of the distance from equilibrium may be found. For instance, for our oscillators one can propose the following approaches:

(i) the norm of the function U_1 which expresses the deviation from the "equilibrium" probability distribution;

(ii) the mean energy of the oscillations;

(iii) the renormalized intensity of the given noise which is the solution of (14*) in this special case.

Both the latter functions are increasing monotonously with increasing excitation in the case of only one pumping parameter.

5. Selforganization in Systems with Two Control Parameters

Selforganization processes are often considered as a sequence of nonequilibrium phase transitions induced by external flows. In this process the control parameters change continuously. However one should not forget that real systems permit such change only in certain parameter ranges.

In the case of one pumping parameter the evolution can go in one direction only. But in the presence of a second one the system can "choose" its evolution-path in the parameter space in the permitted range. However, in any case the most advantageous state is the state with the highest order, hence with the minimal entropy. The change of entropy depends only on the starting and the final point, but not on the pathway between them. Choosing a certain path in the parameter space the evolution process can satisfy some additional conditions. There may be, for instance, conditions on the behaviour of the entropy between both fixed states as well as on the behaviour of some other variables.

Of special interest is the possibility to control the evolution artificially by means of regulating the pumping parameters. This allows to optimate the structure of the system according to one or another criterion. Let us consider an example.

On Fig. 5 a_1 and a_2 are control parameters, Γ is the boundary of the parameter range. "0" is the starting point, for instance the "equilibrium", the family of curves mark constant entropy values. We assume that the entropy has its minimum at the boundary,



Fig. 5. Range in which the control parameters a_1 and a_2 can change continuously. "P" corresponds to minimal entropy, dashed lines to certain evolution pathways

in the point P and does not have any local extremum inside the range. Then we can propose the following criteria for the pathway of the evolution starting from "0" inside the range:

1. The path L turns the integral $I = \int_{0}^{p} (a_1, a_2) \tilde{S} dl(L)$ into minimum that means

a minimization of the path-length under the condition that the system prefers the ranges of lower entropy.

2. The pathway l_1 is directed by the gradient of entropy. Its direction in the starting point follows the maximum concentration of isoentropy curves. The boundary is not reached in "P". Further evolution to "P" is possible along the boundary.

3. The path l_2 coincides with the gradient of entropy too, it starts in "0", however, in such a direction that the boundary is reached in "P".

4. The system comes to the boundary again in "P", but the path is defined by the condition of minimal energy expenditure of the pumping source.

5. The choice of the final point is concerned with extremal conditions on certain other variables, for instance the amplitude of the selfoscillations.

As we have mentioned the proposed approaches should only illustrate the varity of possibilities. Since there is not any experimental data in this field we studied the approaches 1-3 for the simplest dissipative structure with two control parameters, VAN DER POL oscillators.

6. Results of the Computer Calculations

For the systems (1), (4) as well as (9) for given noise we calculated the "mean energy" (15) and the entropy (16)

$$\langle H \rangle = \int dx \, dv \, H(x, v) \, f(x, v) \,, \tag{15}$$

$$\tilde{S}/k = -\int dx \, dv \ln \tilde{f}(x,v) \cdot \tilde{f}(x,v), \quad \tilde{f} \equiv f|_{D=\tilde{D}}, \quad (16)$$

 $D[U_1]$ is the solution of the equation $\langle H \rangle [U_1] |_{D=\tilde{D}} = \text{const.}$

The distribution functions and the "effective Hamiltonian" are defined in (7^*) and (12). Figs. 6 and 7 show the results for the oscillator with a resonance force, Figs. 8–11 for the oscillator with linear and nonlinear feedbacks. In Figs. 6, 8, 10 the results are given for the lowering of the entropy from the "equilibric" level as a function of the two parameters. The bifurcation lines a = 0 or respectively $a = b^2/4c$ are also given. Dashed lines mark, qualitatively only, the paths of selforganization corresponding to the first three approaches. The point of the minimal entropy "P" was chosen arbitrarly, since the boundaries of the parameter ranges are defined by the concrete system. Figs. 7, 9, 11 show the lines of constant "mean energy" values. We obtained the following:

1. Entropy changes rather weakly. The "equilibrium" value S_0/k is of the order of one. In all cases the entropy has its maximum in "equilibrium", in "0" (GIBBS theorem). The isoentropy lines lie around "0". Moving away from "0" in any direction where one parameter is constant, the entropy is decreasing monotonously (S-theorem for the one parameter case). By variations of the second parameter one has the opportunity of further decreasing the entropy of the system.

2. The "mean energy" has no extrema inside the range. It also shows monotonous behaviour along any isoparametric line.

3. The figs. 8 and 9 correspond to the systems (1) and (4) with c = 0. The behaviour of the entropy differs essentially from all other studied situations. Most likely, one cannot disregard the presence of the higher nonlinearities.



Fig. 6. Entropy lowering 10³ $\delta \tilde{S}/k$ for (9). a_p is the linear feedback, \bar{X} the amplitude of the resonance force. $\gamma = 2, b_0 = 0.2, \delta \tilde{S} = S_0 - S$



Fig. 7. ''Mean energy'' (15) for (9). $\gamma=2,\,b_0=0.2$



Fig. 8. Entropy lowering $10^3 \delta \tilde{S}/k$ for (1), (4). a_p , b_p linear and nonlinear feedback respectively $\gamma = 2, b_0 = 0.6, c = 0$



Fig. 9. "Mean energy" (15) for (1), (4). $\gamma = 2, b_0 = 0.6, c = 0$

7. Discussion

The subject of this paper is dissipative structures with two control parameters. We investigated the question of the equilibrium state of those systems. We called "equilibrium" the state of zero values of all pumping parameters. We introduced natural noise, in the presence of it a closed system relaxes to the BOLTZMANN-GIBBS distribution function (5). In the case of any other noise the system evolutes to some distribution



Fig. 10. Entropy lowering $10^3 \delta \tilde{S}/k$ for (1), (4). $\gamma = 2, b_0 = 0.6, c = 0.1$



Fig. 11. "Mean energy" (15) for (1), (4). $\gamma = 2, b_0 = 0.6, c = 0$

with a single maximum which is in zero. We defined the distance from "equilibrium" by the entropy, calculated at fixed "mean energy", more precisely, by the lowering of this entropy from the "equilibrium" level. Hence the degree of order in pumped nonequilibrium systems is defined in the same way as is usual for systems at fixed energy since the work of BOLTZMANN. Of course, for special examples there may be other special measures. For VAN DER POL oscillators we compared two measures, entropy and "mean energy". We obtained that they agree well only for high absolute values fo the control parameters.

Our investigation of selforganization processes in systems with two control parameters was based on the statement that for any pumped system the most advantageous state is the state of minimal entropy. In the case of several pumping parameters the system can already "choose" its path of selforganization in the parameter space. Assuming special criteria there follow various results: Modifying the final state of evolution one can optimate the structure, symmetry and other properties. Furthermore, varying the pathway between both the starting and the final points, one can optimate the conditions under which the final state is reached.

Undoubtely this has practical application also. Many technical and, in particular chemical processes today need very large plants which cannot be expanded very much further. It is necessary to increase the efficiency of these processes on the microscopic level. On the other hand there are a lot of striking illustrations of coherence and synchronism in the behaviour of the particles in dissipative as well as in turbulent structures. It leads to exceptionally effective processes on the macroscopic level. Therefore we are sure that both dissipative and turbulent structures will be widely adopted in practice. At that time the optimization of structures according to certain criteria can increase the efficiency of technical processes.

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Notes added in proof

Since we wrote this article a series of papers on this topic has been published. The behaviour of entropy in systems with two control parameters was investigated also by Ebeling, Engel-Herbert and co-workers (see, e.g., [A]) and in other papers of the authors [B-D]. Certain differences in the results are concerned with different approaches in the entropy renormalization. This problem was studied in detail in [D] (see also the references). In [B] the entropy-statement was applied to a simple model which shows intermittend chaos. Similar problems will be studied in subsequent papers.

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