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A Study of Self-Organizing Processes of Nonlinear Stochastic Variables

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A general theory is given for the time evolution of nonlinear stochastic variables $a(t) = \{a_i(t)\}$ whose statistical distribution is changing due to the self-organization of "macroscopic" order. The dynamics of $a(t)$ is conveniently expressed by self-consistent equations for the ensemble average $x(t) = \langle a(t) \rangle$, the supersystem, and for the deviations $\xi(t) = a(t) - x(t)$, the subsystem; the systems are connected to each other by feedback loops in their dynamics. The time dependence of the variance and the correlation function of $\xi(t)$ are studied in terms of relaxation toward local equilibrium under $x(t)$ and dynamical coupling with $x(t)$. A special example shows that the stochastic motions of subsystems are pulled together by the motion of the supersystem through feedback loops, and that this pull-together phenomenon occurs when symmetry-breaking instability exists in nonlinear systems.

KEY WORDS: Nonlinear Brownian motion; self-organization; feedback loop; pull-together phenomenon; transient state; fluctuation renormalization.

1. INTRODUCTION

The existence of hierarchical chain structures is one of the most important features of nature and is observed most clearly in biological systems. Such

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structures arise with respect to amino acids and low molecular weight molecules, proteins and other high polymers, aggregates of high polymers in the form of organelles, cells, tissues, organs, individuals, families or groups, troops or societies, communities, ecosystems, and so on. Fundamental properties common to hierarchical biological systems higher than biopolymers are that they are generally thermodynamically open systems and that feedback loops[1,2] exist between the behavior of the inferior systems (the subsystems) and that of the superior system (the supersystem) composed of the subsystems. The evolution of the supersystem is determined by those of the subsystems in a statistical way and, at the same time, the feedback loops put the subsystems under the control of the supersystem. Such feedback loops give the biological laws characteristic of life phenomena. In fact, this mutual control of the behavior of systems gives a self-regulation mechanism to the dynamics of the hierarchical system against external forces and boundary conditions. The feedback loop in open systems is responsible for the symmetry-breaking instability in the dynamics of the supersystem.[1,2]

A typical example of feedback regulation is observed between the behavior of a human society and that of its members. The society evolves because of its inherent motive force under the control of public opinion and of "macroscopic" boundary conditions, including external forces. On the other side, the behavior and opinions of the members $a_i(t)$ are determined by their inherent motive force $G_i(a_i)$, characteristic of individuals $i = 1, 2, \ldots, N$, the fluctuating force $f_i(t)$ changing the behavior of the ith member in a random way, and the direct and indirect interactions $\{F_{ij}\}$ among the members. The indirect interaction mediated by the society is related to the feedback regulation of public opinion. Generally, the society evolves with space and time scales much larger than those of its members. The collective behavior in a society has been studied by Weidlich,[3] who regards a society as an ensemble of Ising spins. The polarization of public opinion is compared with the appearance of a macroscopic magnetization in the system, which is treated in terms of a Fokker–Planck equation.

More generally, biological systems with feedback loops may be assumed to be kinds of nonlinear and open systems where the statistical distribution and the correlation of variables $\{a_i(t)\}$ belonging to the subsystems are being changed in a cooperative or autocatalytic manner due to the evolution of the supersystem. Therefore, the dynamics of subsystems are controlled by factors affecting the dynamics of the supersystem, such as external forces and boundary conditions to the supersystem.

In the present paper the effect of the evolution of the supersystem on the dynamics of the subsystems will be studied in terms of the moments and the time-correlation function of the stochastic variables describing the behavior of the subsystems. These quantities can be obtained only when the statistical distribution of the variables is known reasonably well. On the other hand,

stochastic variables characterizing the dynamics of nonlinear systems having instability are generally quite different from Gaussian random processes and difficult to obtain in an explicit form. Consequently, the following approximation will be used throughout the present paper.

A stochastic variable $a(t)$ may be decomposed into a deterministic part $y(t)$ and a fluctuating part $z(t)$, for instance, according to Mori's prescription.[4] The distribution function for $z(t)$ will be obtained by solving a proper Fokker–Planck equation. For the sake of convenience, $a(t)$ will be, however, decomposed here into $x(t) = y(t) + \langle z(t) \rangle$ and $\xi(t) = z(t) - \langle z(t) \rangle$, where $\langle\ \rangle$ denotes the statistical average. It may be expected that $\xi(t)$ evolves much more rapidly than $x(t)$ in a number of practical examples. A Gaussian random process may be assumed in such cases for $\xi(t)$ as a first-order approximation, though it is not always applicable to $z(t)$.

General theories have been given by van Kampen,[5] Kubo *et al.*,[6] and Mori[4,7] for the evolution of macroscopic variables in a nonlinear system. On the other hand, we are interested here in subsystems located in nonequivalent positions in a supersystem. Cells in a tissue are typical examples of such subsystems. Furthermore, proteins and other high polymers correspond to subsystems in organelles. Generally speaking, the time dependence of microscopic variables $\{a_i(t)\}$ must be treated in a number of biological problems, which requires a formulation different from the above theories for macroscopic variables. In Section 2, we introduce the fundamental equations used in this paper and discuss the choice of the order parameter characterizing the order in the dynamics of the system. The equation of the order parameter obtained in Section 2 contains moments characteristic of the microscopic fluctuations. The time evolution of moments is discussed in Section 3. Section 4 is devoted to the calculations of the time correlation function and of the kinetic coefficient of the fluctuations for a given value of the order parameter. An application of our theory is given in Section 5, where a model system exhibiting the order–disorder-like transition for certain parameters is analyzed. General considerations are given in Section 6.

2. FUNDAMENTAL EQUATIONS

Let us study the time evolution of a nonlinear many-component system which, because of instability, is not always in a steady state. We shall discuss the case where the behavior of the components can be represented by stochastic variables $a(t) \equiv \{a_i(t): i = 1, 2,..., N\}$, properties of which will be given below. It is assumed that (1) the components are of the same kind and are essentially "microscopic," and (2) the time dependence of the variables $a(t)$ is given by a set of nonlinear stochastic equations,

$$da(t)/dt = -\gamma a(t) + G(a(t)) + F(a(t)) + f(t) \equiv h(a) + f(t) \qquad (1)$$

where γ and $f(t)$ are, respectively, the friction constant giving the dissipation of $a(t)$ and the fluctuating force acting on $a(t)$ due to the interaction of the system with external surroundings which are in a steady state; $G(a(t))$ is the nonlinear force inherent in the system, meaning that the boundary conditions for the system as a nonlinear open system may be included here, and that the interaction force $F(a)$ is caused by the interactions among the stochastic variables in the system. The fluctuating force will be assumed to be a white Gaussian process, i.e.,

$$\overline{f_i(t)} = 0, \qquad \overline{f_i(t) f_j^*(t')} = 2D\,\delta_{ij}\,\delta(t - t') \tag{2}$$

where the asterisk stands for the complex conjugate and the bar over the variables stands for the average with respect to the ensemble of the random variables $f(t)$; D is the "diffusion" constant, and δ_{ij} and $\delta(t)$ denote the Kronecker's δ-symbol and the Dirac δ-function, respectively.

Without loss of generality it may be assumed that time-independent "macroscopic" boundary conditions for the system are set at the initial time $t = 0$. Note that $\bar{a}(t)$ still depends on the initial condition $\bar{a}(0)$, which cannot be specified completely by only the macroscopic conditions, because of nonlinearity. The average of $\bar{a}(t)$ with respect to the initial condition of the ensemble of the system will be called the ensemble average $\langle a(t) \rangle$ of the variables $a(t)$ and denoted by $x(t)$. The ensemble average $x(t)$, the set of $\{x_i(t)\}$, may depend on the subsystems because the boundary conditions exerted on the different subsystems may not be the same.

Now, the variable $a(t)$ will be split into two parts,

$$a(t) = x(t) + \xi(t) \tag{3}$$

where $\xi(t)$ is the fluctuating part, whose ensemble average vanishes. The variable $a(t)$ may be chosen as $x(t) = 0$ in the equilibrium state which appears when $G(a) = 0$. An order parameter representing the order for the dynamics of the variables may be chosen as

$$X(t) = (1/N) \sum_{i=1}^{N} x_i(t) \equiv \langle\langle a(t) \rangle\rangle \tag{4}$$

provided that the system is composed of subsystems which are statistically equivalent. In more general cases $x(t)$ may be regarded as the order parameter. The fluctuating part $\xi(t)$ varies in time due to the interactions of the subsystem with external surroundings and to interactions with other subsystems in the same system. Here a third assumption will be added: The time scale τ_ξ for the change of the fluctuating part $\xi(t)$ is much smaller than that τ_x for the systematic part $x(t)$ or the order parameter $X(t)$. This leads to the result that the statistical distribution of the variable $\xi(t)$ is close to and

differs only slightly from that for local equilibrium for a given value of $x(t)$. The dependence of $\xi(t) = \xi(t; x(t))$ on the evolution of $x(t)$ will be discussed later.

The third assumption limits the applicability of the present theory to phenomena which have stability with respect to a fluctuation $f(t)$. For instance, it cannot be used for the discussion of critical phenomena characterized by the critical slowing down of the fluctuation. In spite of this limitation, a large domain remains for the application of the present treatment, in particular, in biological problems.

Taking the ensemble average of Eq. (1), one finds

$$dx(t)/dt = \langle h(a(t)) \rangle \tag{5}$$

where the function $h(a(t))$ may be expanded in terms of $\xi(t)$ around $h(x(t))$,

$$\langle h(a(t)) \rangle = h(x(t)) + \sum_n \frac{1}{n!} M_n(t) \nabla^n h(x(t)) \tag{6}$$

where

$$M_n(t) = \langle \xi^n(t) \rangle \tag{7}$$

is the nth moment of ξ. Equations (5)–(7) are written symbolically in such a way as to avoid complexities in the rigorous use of the matrix notation and similar expressions will be used hereafter. Subtracting (5) from (1), one obtains

$$\begin{aligned} \frac{d\xi(t)}{dt} &= h(a) - \langle h(a) \rangle + f(t) \\ &= \sum_n \frac{1}{n!} \{\xi^n(t) - M_n(t)\} \nabla^n h(x(t)) + f(t) \\ &\equiv \Delta h(\xi(t); x(t)) + f(t) \end{aligned} \tag{8}$$

Equations (5) and (8) are different from those in the theories for macroscopic variables; the solution of the deterministic equation, which is independent of the stochastic equation, is chosen as the order parameter in the latter theories, while the order parameter depends explicitly on the stochastic behavior of the subsystems in the present theory. Namely, the equation of motion for $x(t)$ depends on the moments $M_n(t)$ and, at the same time, Eq. (8) depends on $x(t)$. Equation (6) indicates that such a feedback loop exists between $x(t)$ and $\xi(t)$ so far as nonlinearity is present in the system.

The equation of motion for the moment $M_n(t)$ which is derived from Eq. (8) contains M_{n+1}, M_{n+2}, and other higher moments. However, the moments higher than M_2 can be expressed in terms of M_2 because of the third

assumption on the variable $a(t)$, namely the Gaussian distribution of the fluctuation ξ; one finds

$$M_n(t) = \begin{cases} 1 \cdot 3 \cdot 5 \cdots (n-1)[M_2(t)]^{n/2} & \text{for even } n \\ 0 & \text{for odd } n \end{cases} \tag{9}$$

Thus, a closed expression is obtained with respect to $M_2(t)$, the variance.

The time evolution of $\xi(t; x(t))$ may be classified as follows by utilizing the relation $\tau_\xi \ll \tau_x$: (1) $\xi(t)$ relaxes toward the local equilibrium for a given value of $x(t)$, and (2) there is dynamical coupling between $\xi(t)$ and $x(t)$ due to the evolution of $x(t)$. Generally speaking, the dynamical coupling may be characterized by the time scale τ_x and the relaxation by τ_ξ. The description of the time evolution of the moment becomes complex when the relaxation is included explicitly in the treatment, because the relaxation process is composed of a number of "normal modes" and, moreover, there are interferences between the dynamical coupling process and these normal modes.

3. THE TIME DEPENDENCE OF THE VARIANCE

Let us study the evolution of the system in the time interval from t to $t + s$ with the choice of the time scale as $\tau_\xi \ll s \ll \tau_x$, which allows us to discuss the relaxation process explicitly and to study the dynamical coupling by a slight change in the value of $x(t)$. The variance M_2 may be rewritten as

$$\begin{aligned} M_2(t+s) &= M_2(t+s; x(t+s)) \\ &\simeq M_2(t+s; x(t)) + \Delta x(s; t)\, \nabla_x M_2(t+s; x(t)) \\ &\simeq M_2^\circ(t) + \Delta x(s; t)\, \nabla_x M_2^\circ(t) \end{aligned} \tag{10}$$

where $M_2^\circ(t) \equiv M_2(t+\infty; x(t))$ and $\nabla_x M_2^\circ(t) \equiv \nabla_x M_2(t+\infty; x(t))$ are given in the last equation by utilizing $s \gg \tau_\xi$ and hereafter the superscript $^\circ$ on variables indicates that the variables are in local equilibrium for the order parameter fixed at $x = x(t)$. The second term on the rhs of (10) represents the dynamical coupling caused by a slight change $\Delta x(s)$ of x from $x = x(t)$; $\Delta x(s; t)$ is obtained from Eqs. (5) and (6).

The time dependence of the variance in the scale s is given from Eq. (10) as

$$\frac{\partial}{\partial s} M_2(t+s) = \left\{ \frac{\partial}{\partial s} x(s; t) \right\} \nabla_x M_2^\circ(t) \tag{11}$$

The variance $M_2^\circ(t)$ in local equilibrium, which is a steady state value over

the time scale s for a given $x(t)$, may be obtained from

$$\frac{d}{ds} M_2^\circ(t+s) = \left\langle \left\{ \frac{d}{ds} \xi^\circ(t+s) \right\} \xi^{\circ *}(t+s) \right\rangle + \left\langle \xi^\circ(t+s) \frac{d}{ds} \xi^{\circ *}(t+s) \right\rangle = 0 \tag{12}$$

where the second term on the rhs is the complex conjugate (c.c.) of the first term, which may be calculated as follows.

The nonlinear Markov equation

$$d\xi^\circ(t+s)/ds = \Delta h^\circ(\xi^\circ(t+s)) + f(t+s) \tag{13}$$

may be rewritten in terms of a linear non-Markov one by utilizing Mori and Fujisaka's identity.[8] Let $W_t(\xi, s)$ be the probability distribution function of ξ at time $t+s$ for a given $x(t)$. The Fokker–Planck equation corresponding to Eq. (13) is

$$\frac{\partial}{\partial s} W_t(\xi^\circ, s) = -\frac{\partial}{\partial \xi^\circ} (\Delta h^\circ W_t) + D \frac{\partial^2}{\partial \xi^{\circ 2}} W_t \equiv \Pi_t W_t \tag{14}$$

By introducing the adjoint operator Λ_t of Π_t such that

$$\int A(\xi^\circ) \Pi_t W_t(\xi^\circ, s)\, d\xi^\circ = \int \{\Lambda_t A(\xi^\circ)\} W_t(\xi^\circ, s)\, d\xi \tag{15}$$

or

$$\Lambda_t = \Delta h^\circ(\xi^\circ) \frac{\partial}{\partial \xi^\circ} + D \frac{\partial^2}{\partial \xi^{\circ 2}} \tag{16}$$

Eq. (13) can be rewritten as

$$\frac{d}{ds} \xi^\circ(t+s) = \Lambda_t \xi^\circ(t+s) + f(t+s) \tag{17}$$

The function $A(\xi)$ in Eq. (15) is an arbitrary function of ξ. The formal integration of Eq. (17) results in

$$\xi^\circ(t+s) = [\exp(\Lambda_t s)] \xi^\circ(t) + \int_0^s \{\exp[\Lambda_t(s-s')]\} f(t+s')\, ds' \equiv \xi_0^\circ(t+s) + \xi_1^\circ(t+s) \tag{18}$$

The time evolution of the systematic part $\xi_0(t+s)$ of $\xi(t+s)$,

$$\frac{d}{ds} \xi_0^\circ(t+s) = \Lambda_t \xi_0^\circ(t+s) \tag{19}$$

can be transformed into a linear non-Markov equation[9]

$$\frac{d}{ds}\xi_0^\circ(t+s) = i\Omega_t\xi_0^\circ(t+s) - \int_0^s \psi_t(s')\xi_0^\circ(t+s-s')\,ds' + g(t+s) \tag{20}$$

where

$$i\Omega_t \equiv \langle \Delta h^\circ(\xi^\circ(t))\xi^\circ(t)^*\rangle\langle|\xi^\circ(t)|^2\rangle^{-1} \tag{21}$$

$$g(t+s) \equiv \{\exp[(1-P_t)\Lambda_t s]\}(1-P_t)\Lambda_t\xi^\circ(t) \tag{22}$$

$$P_t A \equiv \langle A\xi^{\circ *}(t)\rangle\langle|\xi^\circ(t)|^2\rangle^{-1}\xi^\circ(t) \tag{23}$$

and

$$\psi_t(s) \equiv \langle g(t+s)g(t)^*\rangle\langle|\xi^\circ(t)|^2\rangle^{-1} \tag{24}$$

The definition of the projection operator P_t is different from that given by Mori and Fujisaka in that P_t here is a slowly varying function of time with time scale τ_x and the average is taken with respect to the steady probability distribution of ξ under a given value of $x(t)$.

Since Eq. (20) is a linear equation in $\xi_0^\circ(t+s)$, the corresponding equation for $\xi^\circ(t+s)$ leads to

$$\frac{d\xi^\circ(t+s)}{ds} = i\Omega_t\xi^\circ(t+s) - \int_0^s \psi_t(s')\xi^\circ(t+s-s')\,ds' + g(t+s) + f(t+s) \tag{25}$$

Multiplying by $\xi^{\circ *}(t+s)$ on the right of (25) and taking the ensemble average, one finds

$$\left\langle \left\{\frac{d}{ds}\xi^\circ(t+s)\right\}\xi^{\circ *}(t+s)\right\rangle = i\Omega_t\langle|\xi^\circ(t+s)|^2\rangle - \int_0^s \psi_t(s')\langle\xi^\circ(t+s-s')\xi^{\circ *}(t+s)\rangle\,ds' + \langle g(t+s)\xi^{\circ *}(t+s)\rangle + \langle f(t+s)\xi^{\circ *}(t+s)\rangle \tag{26}$$

The last term in Eq. (26) does not always vanish. In fact, an explicit calculation gives $\langle f(t+s)\xi^{\circ *}(t+s)\rangle = D$, which means that the variance increases due to the "diffusion" of ξ° under the perturbation of $f(t)$. The third term on the rhs of Eq. (26) may be explicitly calculated as follows. The variable $\xi_0^\circ(t+s)$ may be split into two parts as

$$\xi_0^\circ(t+s) = P_t\xi_0^\circ(t+s) + (1-P_t)\xi_0^\circ(t+s) \equiv C_t^\circ(s)\xi^\circ(t) + \eta(t+s) \tag{27}$$

where $C_t^\circ(s)$ is a time correlation function of $\xi(t)$ for a fixed $x(t)$,

$$C_t^\circ(s) \equiv \langle\xi_0^\circ(t+s)\xi^\circ(t)^*\rangle\langle|\xi^\circ(t)|^2\rangle^{-1} \tag{28}$$

Operating with $(1 - P_t)$ from the left on Eq. (19) and substituting Eq. (27), one obtains

$$\partial\eta(t + s)/\partial s = (1 - P_t)\Lambda_t\{C_t^\circ(s)\xi^\circ(t) + \eta(t + s)\} \tag{29}$$

which is easily integrated as

$$\begin{aligned}\eta(t + s) &= \int_0^s \{\exp[(1 - P_t)\Lambda_t(s - s')]\}(1 - P_t)\Lambda_t C_t^\circ(s')\xi^\circ(t)\, ds' \\ &= \int_0^s C_t^\circ(s')g(t + s - s')\, ds'\end{aligned} \tag{30}$$

From the definition (22) of $g(t + s)$, it is easily seen that

$$\langle g(t + s)\xi^{\circ *}(t)\rangle = 0 \tag{31}$$

Therefore, by using Eqs. (24), (28), and (30), we find the third term on the rhs of Eq. (26) to be

$$\begin{aligned}\langle g(t + s)\xi^{\circ *}(t + s)\rangle &= \langle g(t + s)\eta(t + s)^*\rangle \\ &= \int_0^s \langle g(t + s)g^*(t + s - s')\rangle C_t^{\circ *}(s')\, ds' \\ &= \int_0^s \psi_t(s')\langle\xi^\circ(t)\xi^{\circ *}(t + s')\rangle\, ds'\end{aligned} \tag{32}$$

The third assumption on $a(t)$ gives rise to

$$\langle\xi^\circ(t)\xi^{\circ *}(t + s')\rangle = \langle\xi^\circ(t + s - s')\xi^{\circ *}(t + s)\rangle \tag{33}$$

Hence, the third term on the rhs of (26) cancels the second, reducing Eq. (26) to

$$\left\langle\left\{\frac{d}{ds}\,\xi^\circ(t + s)\right\}\xi^{\circ *}(t + s)\right\rangle = i\Omega_t\langle|\xi^\circ(t + s)|^2\rangle + D \tag{34}$$

The steady state variance M_2° is obtained as the solution of

$$i\Omega_t M_2^\circ + M_2^\circ(i\Omega_t)^* + 2D = 0 \tag{35}$$

which is obtained from Eqs. (12) and (34). In (35), $i\Omega_t$ is a function of M_2° and its explicit form depends on $h(a)$.

The effect of the dynamical coupling with increasing $|x|$ on the evolution of the variance depends on the sign of $\nabla_{|x|}M_2^\circ(t)$. The "microscopic" motion of subsystems may be pulled together and reduced by the dynamical coupling, provided that $\nabla_{|x|}M_2^\circ(t) < 0$.

4. THE TIME CORRELATION FUNCTION

The normalized time correlation function $C(s)$ may be written as

$$\begin{aligned}C(s) &\equiv \langle\xi(t + s)\xi^*(t)\rangle\langle|\xi(t)|^2\rangle^{-1} \\ &\simeq C^\circ(s) + \Delta x(s; t)\,\nabla_x C^\circ(s)\end{aligned} \tag{36}$$

where the first term on the rhs represents the correlation of the fluctuation ξ with the order parameter fixed at $x(t)$ and the second term represents the increase or the decrease of the correlation by the dynamical coupling between $\xi(t)$ and $x(t)$. To calculate $C^\circ(s)$, (25) may be utilized. Multiplying Eq. (25) by $\xi^{\circ *}(t)$ from the left and then taking the average, one is left with

$$dC^\circ(s)/ds = i\Omega_t C^\circ(s) - \int_0^s \psi_t(s')C^\circ(s - s')\, ds' \tag{37}$$

The solution of (37) is found in the form of the Laplace transform as

$$C^\circ(z) = [z - i\Omega_t + \psi_t(z)]^{-1} \tag{38}$$

where

$$C^\circ(z) \equiv \int_0^\infty C^\circ(s)e^{-zs}\, ds \tag{39}$$

The frequency-dependent "kinetic coefficient" $\Gamma(\omega)$, e.g., the friction coefficient, is obtained as

$$\Gamma(\omega) = \mathrm{Re}[-i\Omega_t + \psi_t(i\omega)] \tag{40}$$

where Re stands for the real part.

Though the explicit form of the memory function $\psi_t(s)$ is unknown, its approximate form may be calculated as follows in a second-order perturbation expression.[8,10] The evolution operator Λ_t may be split into two parts, one linear and one nonlinear, as

$$\Lambda_t = \Lambda_0 + \Lambda_1 \tag{41}$$

where

$$\Lambda_0 \equiv \{P_t\, \Delta h^\circ(\xi^\circ)\} \frac{\partial}{\partial \xi^\circ} + D \frac{\partial^2}{\partial \xi^{\circ 2}} \tag{42}$$

and

$$\Lambda_1 \equiv \{(1 - P_t)\, \Delta h^\circ(\xi^\circ)\} \frac{\partial}{\partial \xi^\circ} \tag{43}$$

If the nonlinear fluctuation $(1 - P_t)\, \Delta h^\circ(\xi^\circ)$ is small enough, the memory function may be approximated as

$$\begin{aligned} \psi_t(s) &= \langle \{e^{(1-P_t)\Lambda_t s} g(t)\} g^*(t) \rangle \langle |\xi^\circ(t)|^2 \rangle^{-1} \\ &\simeq \langle \{e^{(1-P_t)\Lambda_0 s} g(t)\} g^*(t) \rangle \langle |\xi^\circ(t)|^2 \rangle^{-1} \end{aligned} \tag{44}$$

By using the approximation (44) for $\psi_t(s)$, one is able to express the memory function explicitly in terms of known quantities. For example, if $\Delta h^\circ(\xi^\circ)$ is expressed as

$$\Delta h^\circ(\xi^\circ) = -\gamma \xi^\circ + \alpha\{\xi^{\circ 2} - M_2^\circ\} \tag{45}$$

the random force g is obtained from Eqs. (22) and (45) as

$$g(t) = \alpha\{\xi^{\circ 2}(t) - M_2^{\circ}(t)\} \tag{46}$$

Since the linear part of the evolution operator Λ_t in this case is

$$\Lambda_0 = -\gamma\xi^{\circ}\frac{\partial}{\partial\xi^{\circ}} + D\frac{\partial^2}{\partial\xi^{\circ 2}} \tag{47}$$

a straightforward calculation results in

$$(1 - P_t)\Lambda_0 g = -2\alpha\gamma g - 2\alpha\gamma M_2^{\circ} \tag{48}$$

Thus the second-order perturbation calculation leads to

$$\psi_t(s) \simeq e^{-2\gamma s}\langle|g|^2\rangle\langle|\xi^{\circ}|^2\rangle^{-1} \tag{49}$$

The effect of the dynamical coupling on the correlation function of $\xi(t)$ with increasing $|x|$ is seen qualitatively from the sign of $\nabla_{|x|}C^{\circ}(s)$. As far as the present approximation is concerned, the condition of the self-organization of order, the condition of the pull-together of randomness, in the evolution of stochastic systems may be represented by the decrease of the randomness and the increase of the damping in the fluctuation $\xi^{\circ}(s)$ around the averaged change $x(t + s)$. The former gives a decrease in the variance $M_2^{\circ}(s)$ and the latter a decrease in the correlation function $C^{\circ}(s)$ by the dynamical coupling with increasing $|x|$. Hence, the condition for the pull-together is given by

$$\nabla_{|x|}M_2^{\circ}(s) < 0, \qquad \nabla_{|x|}C^{\circ}(s) < 0 \tag{50}$$

5. A SPECIAL EXAMPLE

The theory developed above will be applied to a system with

$$F_i(a) = \frac{\theta}{N}\sum_j (a_j - a_i), \qquad \theta \geqslant 0 \tag{51}$$

and

$$-\gamma a_i + G_i(a) = pa_i - qa_i^3, \qquad q \geqslant 0 \tag{52}$$

Interactions such as (51) are able to lead to an empirical equation for muscle contraction.[11] It is known that muscle contraction is caused by the mutual sliding of myosin and actin filaments, that there are cross-bridges between myosin and actin extending from a myosin filament toward actin filaments around it, and that the motive force for the sliding arises between the terminal part of the cross-bridge and actin in a repeating manner during muscle contraction. Thus, the molecular dynamics at each cross-bridge may be assumed to be the subsystem and the sliding motion of the filaments as the supersystem. The motive force at the cross-bridge comes from the use of chemical

energy obtained from the hydrolysis of ATP molecule and may be tentatively given by (52). Even if no direct interaction exists between cross-bridges, the motion of one cross-bridge is affected by all others through the sliding motion of the muscular filaments. This sort of interaction may be written as in (51).

For the sake of simplicity we assume that the system is so homogeneous that the order parameter can be chosen as (4). Fundamental equations corresponding to Eqs. (5) and (8) are obtained as

$$dX/dt = pX - qX^3 - 3qXM_2 \tag{53}$$

and

$$d\xi/dt = (p - 3qX^2 - \theta)\xi - 3qX(\xi^2 - M_2) - q\xi^3 + f \tag{54}$$

The evolution of $X(t)$ is not only determined by $X(t)$ itself but also by $\xi(t)$ through the variance $M_2(t)$. Linearizing (54) for a fixed value of $X(t)$, one finds

$$\frac{d\xi^\circ(t+s)}{ds} = i\Omega_t\xi^\circ(t+s) - \int_0^s \psi_t(s')\xi^\circ(t+s-s')\,ds' + g(t+s) + f(t+s) \tag{55}$$

where explicit calculations give

$$i\Omega_t = p - 3qX(t)^2 - \theta - 3qM_2{}^\circ(t) \tag{56}$$

$$g(t+s) = e^{(1-P_t)\Lambda_t s}[-3qX(t)\{\xi^\circ(t)^2 - M_2{}^\circ(t)\} - q\{\xi^\circ(t)^2 - 3M_2{}^\circ(t)\}\xi^\circ(t)] \tag{57}$$

and

$$\Lambda_t = [\{p - 3qX(t)^2 - \theta\}\xi^\circ(t) - 3qX(t)\{\xi^\circ(t)^2 - M_2{}^\circ(t)\} - q\xi^\circ(t)^3]\frac{\partial}{\partial\xi^\circ} + D\frac{\partial^2}{\partial\xi^{\circ 2}} \tag{58}$$

It should be noted here that the interaction force (51) does not appear explicitly in the equation of the order parameter X, Eq. (53). The interaction force influences $X(t)$ indirectly through the θ dependence of the variance of M_2. The steady-state variance corresponding to the order parameter $X(t)$ is easily obtained from Eqs. (35) and (56) as

$$M_2{}^\circ(t) = \{(p - \theta - 3qX^2) + [(p - \theta - 3qX^2)^2 + 12qD]^{1/2}\}/6q \tag{59}$$

It is easily seen from (53) that one of the steady states of the order parameter exists at $X = 0$, indicating a disordered state for $\{a_i\}$, and other steady states are given by the relation

$$p - 3qM_2{}^\circ - qX_0{}^2 = 0 \tag{60}$$

Substituting (59) into (60) and solving the resulting equation, one obtains

$$X_0 = \pm\{2p - \theta + [(2p + \theta)^2 - 24qD]^{1/2}\}^{1/2}/2\sqrt{q} \tag{61}$$

The stability of these steady states is seen from the linear stability analysis: The steady state $X = 0$ is stable for $p\theta < 3qD$ and it becomes unstable for $p\theta > 3qD$, where the steady states (61) are stable. The condition $p\theta = 3qD$ gives marginal stability (Fig. 1).

The memory function $\psi_t(s)$ in (55) may be calculated explicitly by the use of the second-order perturbation approximation (44). The linear part Λ_0 of the evolution operator Λ, Eq. (58), is obtained from (42) and (58) as

$$\Lambda_0 = [(p - 3qX^2 - \theta)\xi^\circ - 3qM_2{}^\circ\xi^\circ]\frac{\partial}{\partial\xi^\circ} + D\frac{\partial^2}{\partial\xi^{\circ 2}} \tag{62}$$

The approximation

$$g(t + s) = e^{(1-P_t)\Lambda_0 s}g(t) \tag{63}$$

and the expression (57) for g yield

$$\begin{aligned}\dot{g} &= (1 - P_t)\Lambda_0 g \\ &= 3(p - 3qX^2 - \theta - 3qM_2{}^\circ)[g + qX(\xi^{\circ 2} - 3M_2{}^\circ)]\end{aligned} \tag{64}$$

after simple calculations. From Eqs. (64) and (56) one obtains

$$\begin{aligned}g(t + s) = {} & [\exp(3i\Omega_t s)]g(t) \\ & + \int_0^s \{\exp[3i\Omega_t(s - s')]\}3i\Omega_t qX(t)\{\exp[(1 - P_t)\Lambda_0 s']\} \\ & \times \{\xi^{\circ 2}(t) - 3M_2{}^\circ(t)\}\, ds'\end{aligned} \tag{65}$$

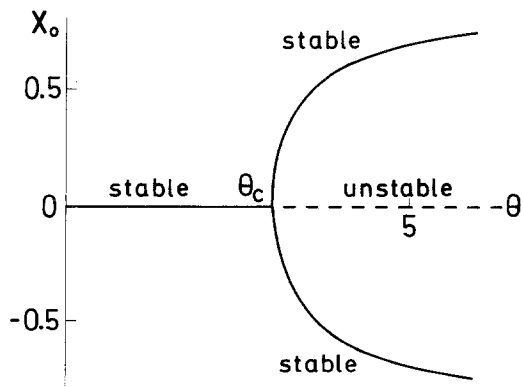

Fig. 1. Steady state for X for a system represented by (53) for $p = q = D = 1.0$. Here θ_c is the critical strength for the appearance of the order, $\theta_c = 3qD/p$. A similar figure is obtained for X vs. p for fixed q and θ.

Similar calculations result in

$$\{\exp[(1 - P_t)\Lambda_0 s]\}\{\xi^{\circ 2}(t) - 3M_2^{\circ}(t)\}$$
$$= 3[\exp(2i\Omega_t s) - 1] + [\exp(2i\Omega_t s)]\{\xi^{\circ 2}(t) - 3M_2^{\circ}(t)\} \tag{66}$$

The memory function becomes

$$\psi_t(s) = [\exp(3i\Omega_t s)]\psi_t(0) - 18i\Omega_t q^2 M_2^{\circ}(t)^2 X(t)^2 \times \int_0^s \exp[3i\Omega_t(s - s')] \exp(2i\Omega_t s')\, ds' \tag{67}$$

from Eqs. (65)–(67) and (44). By using (40) and (67), we find the kinetic coefficient $\Gamma(\omega)$ for a given value of $X(t)$ as

$$\Gamma(\omega; X(t)) = \mathrm{Re}\left[-i\Omega_t + \frac{\psi_t(0)}{i\omega - 3i\Omega_t} - \frac{18i\Omega_t q^2 M_2^{\circ}(t)^2 X(t)^2}{(i\omega - 3i\Omega_t)(i\omega - 2i\Omega_t)}\right] \tag{68}$$

The variance M_2° and the kinetic coefficient Γ are independent of X when $q = 0$, i.e., when the system is linear: For $\theta > p$

$$M_2^{\circ} = D(\theta - p) \tag{69}$$

and

$$\Gamma = \theta - p \tag{70}$$

as is easily seen by taking the limit $q \to 0$ in (59) and (68). The evolution of the order parameter $X(t)$ is given in closed form as

$$\dot{X}(t) = pX(t) \tag{71}$$

in which no information on $\xi(t)$ is contained.

For $q \neq 0$ both the variance M_2° and the kinetic coefficient depend on

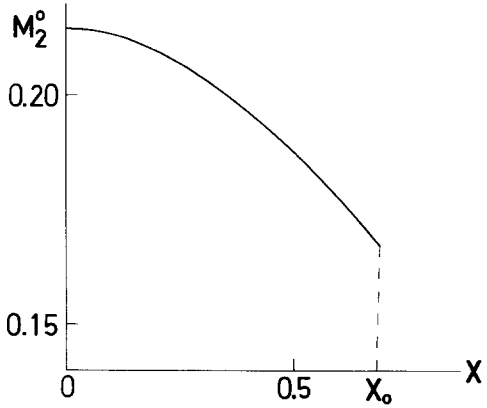

Fig. 2. The dependence of the variance on X, Eq. (59), for $p = q = D = 1.0$ and $\theta = 5.0$. X_0 is the steady-state value of X for given values of p, q, and θ, $X_0 = 0.707$.

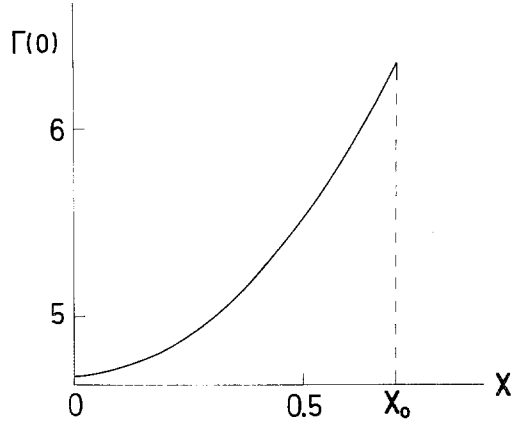

Fig. 3. The dependence of the kinetic coefficient Γ on X, Eq. (68), for $\omega = 0$, $p = q = D = 1.0$, and $\theta = 5.0$. Similar curves are obtained for arbitrary frequencies.

the order parameter X, and are shown in Figs. 2 and 3. As is seen from these figures, their derivatives with respect to $|X|$ are

$$\partial M_2^{\circ}(t; X)/\partial |X| < 0 \tag{72}$$

and

$$\partial \Gamma(\omega; X)/\partial |X| > 0 \qquad \text{for all} \quad \omega \tag{73}$$

Thus, due to the dynamical coupling, the variance becomes smaller and smaller as order develops in the system, while the kinetic coefficient becomes larger and larger over the whole frequency region. In other words, the system satisfies the condition of pull-together, Eq. (50). The decrease in the variance influences the evolution of the order parameter through a feedback loop, namely, the growth rate of $X(t)$, $p - 3qM_2^{\circ}$ in (53), becomes larger as the variance becomes smaller. Because of the feedback loop, macroscopic order develops more and more in the system as the fluctuation around it is reduced more and more by the increasing order parameter. At the same time the kinetic coefficient, which becomes larger, pulls back the deviation of $a(t)$ from $X(t)$ more rapidly.

6. DISCUSSION

A fundamental property common to self-organizing systems is the existence of feedback loops between macroscopic and microscopic behaviors in the system. The necessary condition for such a feedback regulation of hierarchical systems is evidently the existence of nonlinearity in the dynamics of the system. In fact, when $q = 0$, i.e., when the system is linear, the evolution of the order parameter $X(t)$ is determined only by $X(t)$, as shown in (71). The

corresponding steady state at $X = 0$ is unstable, provided that $p > 0$. However, the variance given by (69) is constant and independent of X regardless of the sign of p. In other words, even if the order parameter evolves, the fluctuation $\xi(t)$ is not controlled by $X(t)$, because of the lack of a feedback loop in the linear system. It is immediately clear from this fact that the pull-together effect of $\xi(t)$ occurs only in nonlinear systems through the dynamical coupling.

In the model discussed in Section 5 the kinetic coefficient for a given value of $X(t)$ becomes larger and larger as order develops in the system. This phenomenon may be generalized for the self-organizing system as discussed by Shimizu[12]: The effective potential for microscopic variables grows during the evolution of the order parameter and the deviation from the organizing motion is pulled back stronger and stronger by the effective potential.

The kinetic coefficient in Section 5 is of a second-order perturbation approximation. As is shown by Kawasaki,[13] one possible way to avoid the perturbation calculation is to find a closed form for $C^\circ(t)$ in (37) by simply assuming that the time-evolution operator $\exp\{(1 - P_t)\Lambda_t s\}$ in $\psi_t(s)$ can be replaced by $\exp(\Lambda_t s)$ and the resulting many-body correlations of $\xi^\circ(s)$ by the products of $C^\circ(s)$.

A dynamical coupling between the time-dependent average of stochastic quantities and the fluctuations also was studied by Nordholm and Zwanzig.[14] They have shown how the fluctuation renormalization can be obtained exactly by a formal procedure and approximately by more tractable methods. However, no explicit dependence of the variance on x is considered in their theory.

The ensemble average discussed in Section 2 cannot always be calculated for nonphysical phenomena. For example, in the statistical development of a human society only one sample is available and it might seem insufficient to discuss the probability distribution for such a system. Nevertheless, the present theory may be applied to such a system if the number of members of the system is sufficiently large, for the reason discussed by Weidlich[3] in his interesting study of the mass-opinion-forming process in a human society; namely, the probability distribution is sharply enough peaked with respect to the relevant variables that the possible deviations from their mean values are very small in every sample.

7. CONCLUSION

The statistical distribution of nonlinear stochastic variables, the "microscopic" variables $a(t) = \{a_i(t)\}$, varies with time as the self-organization of order advances at the "macroscopic" level in the system of the variables. The process of order formation in such a stochastic system is conveniently discussed in terms of the hierarchical structure of the system as long as the

number of variables is large enough and the state of the system is not very close to a critical one: The whole system is decomposed into a supersystem of "macroscopic" size and subsystems of "microscopic" size. The time evolution of these hierarchical systems is controlled by dynamical feedback loops. More concretely, the "macroscopic" variable or the order parameter $x(t)$ characterizes the order formed in the system at the macroscopic level and therefore, belongs to the supersystem. The fluctuations of the variables around the ordered evolution $x(t)$, e.g., $\xi(t) = a(t) - x(t)$, characterize the local behavior of the subsystems. Therefore, they are regarded as microscopic quantities. From a nonlinear Langevin equation for $a(t)$ a set of equations for $x(t)$ and $\xi(t)$ is obtained. The "deterministic" equations for $x(t)$ depend on $\xi(t)$ through the variance of $\xi(t)$ under the Gaussian approximation for $\xi(t)$, and the "kinetic coefficient" or the "effective potential" for $\xi(t)$ in the stochastic equations of the subsystems is an increasing function of $|x(t)|$. Thus, these two kinds of equations should be solved in a self-consistent way. Qualitatively, the evolution of $\xi(t)$ for a short time can be decomposed into relaxation toward local equilibrium for a "fixed" value of order parameter and dynamical coupling with the motion of the order parameter through a feedback loop. Indirect interaction between the evolutions of different subsystems comes through dynamical coupling, and a pull-together phenomenon of the evolutions occurs, which leads to the self-organization of order. Mori and Fujisaka's renormalization theory for nonlinear stochastic variables is conveniently used for quantitative calculation of the time dependence of the variance and the correlation function of $\xi(t)$. The self-organization of order by the pull-together phenomenon is represented in terms of a reduction of the variance and an increase in the kinetic coefficient for $\xi(t)$ by dynamical coupling. The feedback loop exists in hierarchical systems only when nonlinearity is present in the dynamics of the variables $a(t)$. The condition for pull-together of random motion is found from the evolution criterion for $x(t)$, and the criterion is determined not only by $x(t)$ but also by $\xi(t)$. Qualitatively, the condition is the existence of symmetry-breaking instability in stochastic systems.

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