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Fluctuation and Relaxation of Macrovariables

Ryogo Kubo,[1] Kazuhiro Matsuo,[1] and Kazuo Kitahara[2]

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Assuming that a macrovariable follows a Markovian process, the extensive property of its probability distribution is proved to propagate. This is a generalization of the Gaussian properties of the equilibrium distribution to nonequilibrium nonstationary processes. It is basically a WKB-like asymptotic evaluation in the inverse of the size of the macrosystem. Evolution of the variable along the most probable path and fluctuation properties around the path are considered from a general point of view with an emphasis on the relation of nonlinearity of evolution and the associated fluctuation. Anomalous behavior of the fluctuation is discussed in connection with unstable, critical, or marginal states. A general treatment is given for the asymptotic properties of relaxation eigenmodes.

KEY WORDS: Relaxation and fluctuation; Markovian process; propagation of extensive property; birth and death process; kinetic Weiss–Ising model; Brownian motion; generalized Fokker–Planck equation; fluctuations far from equilibrium; relaxation spectrum in critical states; path integral.

1. INTRODUCTION

A macrovariable is defined as an extensive quantity describing macrostates of a large system composed of a great number of elementary units interacting with each other and possibly with the environment. Extensive thermodynamic quantities such as the internal energy, the total magnetization, or the number of molecules of a chemical species are examples from statistical

[1] Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo, Japan.
[2] Chimie Physique II, Faculté des Sciences, Université Libre de Bruxelles, Brussels, Belgium.

physics. In nonphysical problems the population of a given sort of group in a society, for example, is considered as a macrovariable. It is a sum-function composed of a great number of microscopic quantities, the statistical average of which is usually considered as a value realized in a given macrostate. Here we regard it as a stochastic variable to include its fluctuation.

In a statistical equilibrium state the distribution of such a macrovariable will be generally nearly normal or Gaussian, the mean square deviations around the average being proportional to the size of the system. In ideal cases of noninteracting units this is proved by the central limit theorem of probability theory. In a system composed of interacting units, in spite of the fact that the central limit theorem has not been proved with such a great generality, the above-mentioned normal property is certainly a very general asymptotic law of a macrovariable, delicate exceptions being reserved for critical situations. Statistical thermodynamics assumes that the statistical distribution of a macrovariable, say X, is given by the law

$$P_e(X) = \text{const} \times \exp \Phi_e(X) = \text{const} \times \exp \Omega\phi_e(x) \tag{1}$$

where $\Phi_e(X)$ is the negative free energy divided by kT and is a function of X and $\phi_e(x)$ is that for a unit volume as a function of the normalized macrovariable,

$$x = X/\Omega \tag{2}$$

Ω being the volume of the system. The most probable value X_e of X (or x_e of x) is determined by maximizing Φ_e (or ϕ_e). Retaining the quadratic term of the expansion of ϕ around the most probable value, the distribution of fluctuations is described by the Gaussian law,

$$\begin{aligned} P_e(X) &= C \exp - \frac{(X - X_e)^2}{2\Omega\sigma_e} \\ &= C \exp \left[- \frac{\Omega}{2\sigma_e} (x - x_e)^2 \right] \end{aligned} \tag{3}$$

It should be kept in mind that the distribution law (1) contains much more information than the Gaussian law, although the deviations from the Gaussian law are of limited interest for most practical purposes. A serious question arises, however, when the system is near a critical point, where the function ϕ_e may lose the analyticity implicitly assumed in the Gaussian approximation.

We now ask ourselves if an asymptotic property of a macrovariable similar to (1) could be assumed in nonequilibrium states of a large system. In other words, the question is whether or not it is possible to describe the temporal evolution of a macrovariable X or a set of such macrovariables by

a distribution function which is a generalization of the asymptotic form (1). At time t this would be of the form

$$P(X, t) = C \exp \Phi(X, t) = C \exp[\Omega\phi(x, t)] \tag{4}$$

If we call the probability distribution for finding X to be X_1 at $t = t_1$, X_2 at $t = t_2$, etc., this would be of the form

$$P(X_1, t_1 ; X_2, t_2 ;...) = C \exp \Omega\phi(x_1, t_1 ; x_2, t_2 ;...) \tag{5}$$

The most probable value of X at t is determined by maximizing the function ϕ in (4). More generally, the most probable evolution of the macrovariable is along the path that maximizes the function ϕ in (5). In the limit of a continuous set of time points the function ϕ is considered as a functional of x_t, which plays a role similar to the action integral. The quadratic expansion around the most probable value or the most probable path will describe the fluctuation as a Gaussian process. Much more information is contained, however, in the function ϕ in (4) or (5).

The general problem we are concerned in this work is thus the asymptotic law of evolution of a macrovariable or a set of macrovariables including fluctuations around a deterministic path. This problem has been studied by van Kampen,[1–3] who developed an expansion method which essentially corresponds to the methods used for proving the central limit theorem. The normalized macrovariable $x(t)$ is assumed to be of the form

$$x(t) = y(t) + \Omega^{-1/2}\xi \tag{6}$$

where ξ is considered as a quantity of the order of Ω^0. Assuming that the variable X follows a Markovian process, he showed that the master equation of the Markovian process can be transformed in an asymptotic limit of a very large size Ω into a generalized Fokker–Planck equation. The most probable path $y(t)$ is determined by a determinstic law of evolution. Kubo[4] has shown that the same results can be directly derived from the Ansatz (4). In the present paper this latter approach will be expounded in greater detail.

In this work we also base our study upon the Markovian assumption. This might seem unsatisfactory from the point of view of the physicist, who would like to start from the very basic dynamic laws at the microscopic level. Leaving such an ambitious attempt for a future project, we wish here to pave the road by attacking the problem in this rather modest approach. We might point out, however, that this approach has its own advantage, because, in a sense, it is more general than a microscopic approach. The microscopic dynamics is certainly a special limit of a Markovian process so that the most essential points may likely remain unaltered when the problem is formulated

in a more general way. A microscopic approach at the present stage would have to use highly complicated, yet not very rigorous techniques. On the other hand, our approach is simpler and transparent, even if it also may not be fully developed in the mathematician's sense. It is not too sensitive to the nature of microscopic dynamics and so it can enjoy some generality. This makes it possible to apply the theory to physical as well as to nonphysical problems of similar nature.

The asymptotic form of Eq. (4) reminds us of the WKB approximation. The parameter of smallness here is

$$\epsilon = \Omega^{-1}$$

which is regarded as the counterpart of the Planck constant h in quantum mechanics. A Schrödinger wave function

$$\psi \sim \exp[(i/\hbar)\, S(x, t)]$$

is compared with (4). Generally speaking, the expansion of $S(x, t)$ in terms of h is not convergent but is only semiconvergent or asymptotic. The same is true for the function $\phi(x, t)$ in Eq. (4). In fact, expression (1) is, as is well known, an asymptotic form obtained, for example, with the use of the Stirling formula or the method of the steepest descent. This asymptotic nature makes the problem hard to handle with mathematical rigor. Here we take a physicist's attitude and try to pursue the problem as far as it seems possible to attain some physically meaningful results.

After defining our problem in Section 2 we shall first show that the use of the asymptotic form (4) is justified in the sense that it propagates. This proof is based upon a simple assumption that elementary changes of the system occur spontaneously with probabilites determined by the internal states of the system. In the course of proof evolution equations are obtained for the cumulants of the probability distribution. In Section 4 these equations are rederived on the basis of the Ansatz (4). The relation of this treatment to van Kampen's method will be commented on. Evolution of the most probable path and the variance of fluctuations around the path are determined by a set of ordinary differential equations. In the case of a single variable the variance at each instant is determined by the value of the macrovariable at the same instant, but if there are many variables the situation is more complex. The limiting law of determinsitic evolution is defined by the average velocity or the first moment of transition probability. The simplest ideal law of such evolution is a linear relaxation, which the classical Brownian motion rigorously follows. It is also realized in the linear regime of a macrovariable in the neighborhood of its equilibrium. If a system is far from equilibrium, the evolution law is generally nonlinear. Fluctuations around such a non-

linear evolution can, however, be described normally as a nonstationary Markovian Gaussian process. From this point of view a path integral representation of the process is presented. A general formula for the correlation function of fluctuations in such a nonlinear nonstationary process is derived. When a system starts from an unstable equilibrium to approach a new stable equilibrium there will be an enormous enhancement of fluctuation or noise appearing in the course of the transition. At a critical or a catastrophic point a Gaussian approximation becomes no longer possible. Relaxation is essentially nonlinear and the phenomena of critical slowing down appear. Correspondingly, fluctuation becomes anomalous. This anomaly is connected with an accumulation of relaxation eigenfrequencies at zero. In the last section a general treatment is given for the eigenmodes of relaxation and eigenfrequencies in order to clarify some aspects of their asymptotic properties.

2. THE MASTER EQUATION

Let X be a macrovariable of a system, the size of which is denoted by Ω. It is assumed to be a stochastic variable following a Markovian process, which is described by the master equation (Chapman–Kolomogorov equation) of the form

$$(\partial/\partial t)\, P(X, t) = -\int W(X \to X', t)\, dX'\, P(X, t) + \int W(X' \to X, t)\, dX'\, P(X', t) \quad (7)$$

where $P(X, t)$ is the probability density of finding X at the value X at the time t and $W(X \to X', t)$ is the transition probability per unit time from X to X'. For simplicity the realized values of X are denoted by the same notation as the random variable itself and are assumed to be continuous. If they are discrete, the integrals are to be replaced by summations. If there exists a set of random variables, X is thought of as a vector. We make here the following two basic assumptions for the transition probability.

(a) A transition of the system is an event that makes X jump by an amount r which may take various values according to the transition probability

$$W(X \to X + r, t) \equiv W(X, r, t) \quad (8)$$

(b) The probability that such a transition takes place in an infinitely short time interval is proportional to its size Ω and is determined by the internal state of the system, so that the function (8) has the form

$$W(X, r, t) = \Omega w(x, r, t) \quad (9)$$

where

$$x = X/\Omega$$

is the normalized intensive macrovariable corresponding to X.

With these assumptions the master equation (7) is written as

$$\epsilon(\partial/\partial t)\, P(x, t) = -\int w(x, r, t)\, dr\, P(x, t) + w(x - \epsilon r, r, t)\, dr\, P(x - \epsilon r, t) \tag{10}$$

for the probability density function $P(x, t)$,

$$P(x, t) = \Omega P(X, t)$$

where the smallness parameter ϵ is

$$\epsilon = \Omega^{-1}. \tag{11}$$

Equation (10) can be written in a formal way as

$$\epsilon \frac{\partial}{\partial t} P(x, t) = -\int dr \left[1 - \exp\left(-\epsilon r \frac{\partial}{\partial x}\right)\right] w(x, r, t)\, P(x, t) \tag{12}$$

or

$$\frac{\partial}{\partial t} P(x, t) = \sum_{n=1}^{\infty} \frac{(-)^n}{n!} \epsilon^{n-1} \left(\frac{\partial}{\partial x}\right)^n c_n(x, t)\, P(x, t) \tag{13}$$

where

$$c_n(x, t) = \int r^n w(x, r, t)\, dr \tag{14}$$

is the nth moment of the transition probability w. We assume the convergence of all moments (14) and the Kramers–Moyal expansion (13). This is certainly a strong assumption, but the task to weaken this is left to the mathematician.

A few examples may serve for illustration. A kinetic Weiss–Ising model[4,5] is defined by the following master equation for the probability $P(N_+, N_-, t)$ of finding N_+ plus and N_- minus spins ($N_+ + N_- = N$) at time t:

$$\begin{aligned}(\partial/\partial t)\, P(N_+, N_-, t) &= -[W_{+-}(N_+, N_- \to N_+ - 1, N_- + 1) \\ &\quad + W_{-+}(N_+, N_- \to N_+ + 1, N_- - 1)]\, P(N_+, N_-, t) \\ &\quad + W_{-+}(N_+ - 1, N_- + 1 \to N_+, N_-)\, P(N_+ - 1, N_- + 1, t) \\ &\quad + W_{+-}(N_+ + 1, N_- - 1 \to N_+, N_-)\, P(N_+ + 1, N_- - 1, t)\end{aligned} \tag{15}$$

where

$$W_{+-}(N_+, N_- \to N_+ - 1, N_- + 1) = N_+ \exp[-\mu - (\alpha/N)(N_+ - N_-)]$$
$$W_{-+}(N_+, N_- \to N_+ + 1, N_- - 1) = N_- \exp[\mu + (\alpha/N)(N_+ - N_-)] \tag{16}$$

are the transition probabilities for the spin flip. A flip of a spin among N_+ plus spins (or N_- minus spins) in a unit time is proportional to N_+ (or N_-) and is assumed to be determined by the exponential Boltzmann factor in which

$$\mu = \mu_0 H/kT, \qquad \alpha = J/kT$$

represent the external magnetic field and the molecular field scaled by kT. Generally the transition probabilities can be more complex, but choosing the rate factor independent of spin configurations (16) is the simplest possible assumption which bears the characteristic features of Ising spins in the Weiss limit in contact with a thermal bath. The transition probabilities assure the equilibrium distribution

$$P_e(N_+, N_-) = \frac{N!}{N_+!\, N_-!} \exp\left[\mu(N_+ - N_-) + \frac{\alpha}{2N}(N_+ - N_-)^2\right] \tag{17}$$

If we write

$$x = (N_+ - N_-)/N$$

Eq. (15) takes the form

$$\begin{aligned} \tfrac{1}{2}\epsilon(\partial/\partial t)\, P(x, t) = &- \tfrac{1}{2}\{e^{-\mu-\alpha x}(1 + x) + e^{\mu+\alpha x}(1 - x)\}\, P(x, t) \\ &+ \tfrac{1}{2}e^{\mu+\alpha(x-\epsilon)}(1 - x + \epsilon)\, P(x - \epsilon, t) \\ &+ \tfrac{1}{2}e^{-\mu-\alpha(x+\epsilon)}(1 + x + \epsilon)\, P(x + \epsilon, t) \end{aligned} \tag{18}$$

or

$$\begin{aligned} \epsilon(\partial/\partial t)\, P(x, t) = &- [(1 - e^{\epsilon(\partial/\partial x)})\, e^{-\mu-\alpha x}(1 + x) \\ &+ (1 - e^{-\epsilon(\partial/\partial x)})\, e^{\mu+\alpha x}(1 - x)]\, P(x, t) \end{aligned} \tag{19}$$

with $\epsilon = 2/N$. The moments of transition probabilities are

$$\begin{aligned} c_n &= 2[-x \cosh(\mu + \alpha x) + \sinh(\mu + \alpha x)] \qquad \text{for odd } n \\ c_n &= 2[\cosh(\mu + \alpha x) - x \sinh(\mu + \alpha x)] \qquad \text{for even } n \end{aligned} \tag{20}$$

If the molecular field coefficient α is put equal to zero, the model represents noninteracting spins. It should be noted that this is equivalent to the Ehrenfest model modified to a continuous-time case.

More generally, the following type of birth and death processes belong to the category of our problem. If $A(X, r, t)$ is the rate of death of r individuals and $B(X, r, t)$ is that of birth of r individuals out of a polulation of X, the master equation for the process will be

$$\begin{aligned}(\partial/\partial t)\, P(X, t) = &- \sum_r A(X, r, t)\, P(X, t) \\ &+ \sum_r A(X + r, r, t)\, P(X + r, t) - \sum_r B(X, r, t)\, P(X, t) \\ &+ \sum_r B(X - r, r, t)\, P(X - r, t) \end{aligned} \tag{21}$$

where $P(X, t)$ is the probability of finding the population to be X at time t. If, further, the rates of birth and death are proportional to the size of the system, as may be assumed in most cases, we put

$$A(X, r, t) = \Omega a(x, r, t), \qquad B(X, r, t) = \Omega b(x, r, t) \tag{22}$$

where $x = X/\Omega$ is the population density. Equation (10) takes the form

$$\begin{aligned}\epsilon(\partial/\partial t)\, P(x, t) = &- \sum_r [a(x, r, t) + b(x, r, t)]\, P(x, t) \\ &+ \sum_r a(x + \epsilon r, r, t)\, P(x + \epsilon r, t) \\ &+ \sum_r b(x - \epsilon r, r, t)\, P(x - \epsilon r, t) \end{aligned} \tag{23}$$

of which the above-mentioned Weiss–Ising model is only a special case. The transition moments are defined by

$$c_n(x, t) = \sum_r r^n[(-)^n a(x, r, t) + b(x, r, t)] \tag{24}$$

The transition probabilities W in Eq. (7) can generally be dependent on time. If, however, the process is stationary and if a unique statistical equilibrium exists, then the transition probabilities are conditioned by this requirement, which, in general, however, is only weak. If the strong condition of detailed balance can be assumed, this gives

$$P_e(X)\, W(X \to X') = P_e(X')\, W(X' \to X) \tag{25}$$

where $P_e(X)$ is the equilibrium probability. This allows us to write the transition probabilities in the form

$$W(X \to X') = \overline{W}(X \mid X')[P_e(X')/P_e(X)]^{1/2} \tag{26}$$

or

$$W(X \to X') = \overline{W}(X \mid X') \exp\{\tfrac{1}{2}[\Phi_e(X') - \Phi_e(X)]\} \tag{27}$$

Here W is symmetric,

$$\overline{W}(X \mid X') = \overline{W}(X' \mid X) \tag{28}$$

and the function $\Phi_e(X)$ is defined by (1). If the variable X is a thermodynamic one, $\Phi_e(X)$ gives

$$(1/\Omega)\,\Phi_e(X) = \phi_e(x) = -\beta f_e(x) \tag{29}$$

in the thermodynamic limit of a large system. The normalized transition probability w in Eq. (10) is then expressed as

$$w(x, r) = \overline{w}(x, r) \exp[\tfrac{1}{2} r(\partial \phi_e/\partial x) + O(\epsilon)] \tag{30}$$

for a jump by r from the state x. The condition (28) means that

$$\overline{w}(x, r) = \overline{w}(x + \epsilon r, -r) \tag{31}$$

or

$$\overline{w}(x, r) = \overline{w}(x, -r) + O(\epsilon) \tag{32}$$

Therefore the moments of transitions are written as

$$c_n(x) = 2 \int_{r>0} dr\, r^n \overline{w}(x, r) \sinh[\tfrac{1}{2} r\, \partial \phi_e/\partial x] + O(\epsilon) \tag{33}$$

for odd n and

$$c_n(x) = 2 \int_{r>0} dr\, r^n \overline{w}(x, r) \cosh[\tfrac{1}{2} r\, \partial \phi_e/\partial x] + O(\epsilon) \tag{34}$$

for even n. Implications of these equations will be discussed later.

3. PROPAGATION OF THE EXTENSIVE PROPERTY OF A MACROVARIABLE

In a previous work by one of the present authors it was assumed as an Ansatz that the transition probability distribution of a macrovariable as determined by Eq. (10) has the asymptotic form

$$P(x, t) = C \exp\{(1/\epsilon)\,[\phi(x, t) + O(\epsilon)]\} \tag{35}$$

This Ansatz can be justified, as will be seen in the following, in the sense that this type of solution of Eq. (10) propagates in time, although it is not unique. If a solution of the equation has this form at an arbitrary initial time, it will keep this form at later times. This assertion may be called the propagation of the *extensive* property of the distribution of a macrovariable. This conservation may possibly be violated when the system changes through a critical point, but with this reservation the theorem can be proved as follows.

Let us introduce the characteristic function $Q(\xi, t)$ defined by

$$Q(\xi, t) = \int P(x, t)\, e^{i\xi x}\, dx \equiv \langle e^{i\xi x} \rangle \tag{36}$$

Then Eq. (12) gives

$$\begin{aligned} \epsilon \frac{\partial}{\partial t} Q(\xi, t) &= -\iint dx\, dr\, e^{i\xi x}(1 - e^{i\epsilon\xi r})\, w(x, r, t)\, P(x, t) \\ &= \iint dx\, dr \int_0^r ds\, i\epsilon\xi e^{i\xi x + i\epsilon\xi s} w(x, r, t)\, P(x, t) \end{aligned} \tag{37}$$

Here we used the formula

$$1 - e^{i\epsilon\xi r} = -\int_0^r ds\, i\epsilon\xi e^{i\xi s}$$

Defining

$$w[\xi, r, t] = \int e^{i\xi x} w(x, r, t)\, dx \tag{38}$$

we have

$$\int dx\, e^{i\xi x} w(x, r, t)\, P(x, t) = (1/2\pi) \int d\eta\, Q(\xi - \eta, t)\, w[\eta, r, t] \tag{39}$$

so that Eq. (37) is written as

$$\frac{\partial}{\partial t} Q(\xi, t) = \frac{1}{2\pi} \int dr \int d\eta \int_0^r ds\, i\xi e^{i\epsilon\xi s} Q(\xi - \eta, t)\, w[\eta, r, t] \tag{40}$$

The solution of this equation is assumed to have the form

$$Q(\xi, t) = \exp q(\xi, t) = \exp \sum_{n=1}^{\infty} [(i\xi)^n/n!]\, q_n(t) \tag{41}$$

which gives

$$Q(\xi - \eta, t) = \exp q(\xi - \eta, t) = \exp \left[\sum_{n=0}^{\infty} (\xi^n/n!)\, q^{(n)}(-\eta, t) \right] \tag{42}$$

with

$$q^{(n)}(-\eta, t) = [(\partial/\partial\xi)^n\, q(\xi, t)]_{\xi=-\eta} \tag{43}$$

if the analyticity of the cumulant function q can be assumed. Inserting

expression (42) into Eq. (40) and dividing both sides of the equation by Q, we get

$$\sum_{n=1}^{\infty} \frac{(i\xi)^n}{n!}\, \dot{q}_n(t) = \frac{1}{2\pi} \int d\eta\, dr \int_0^r ds\, w[\eta, r, t] \exp q(-\eta, t) \times i\xi \exp\left[i\epsilon\xi s + \sum_{n=1}^{\infty} \frac{(i\xi)^n}{n!} h_n(\eta, t)\right] \tag{44}$$

where we introduced the notation

$$h_n(\eta, t) = i^{-n}[q^{(n)}(-\eta, t) - q^{(n)}(0, t)] \tag{45}$$

By Eqs. (41) and (43) this is expressed as

$$h_n(\eta, t) = \sum_{m=1}^{\infty} (1/m!)(-i\eta)^m\, q_{n+m}(t) \tag{46}$$

Now the last exponential function in the integrand of Eq. (44) is expanded into a power series of ξ as

$$\exp\left[i\epsilon s\xi + \sum_{n=1}^{\infty} \frac{(i\xi)^n}{n!} h_n(-\eta, t)\right] = \sum_{n=0}^{\infty} \frac{(i\xi)^n}{n!} m_n(\epsilon, s, \eta, t) \tag{47}$$

Thus Eq. (44) is reduced to the set of equations

$$\frac{1}{n}\, \dot{q}_n(t) = \frac{1}{2\pi} \int d\eta \int dr\, e^{q(-\eta,t)} w[\eta, r, t] \int_0^r ds\, m_{n-1}(\epsilon, s, \eta, t) \tag{48}$$

for $n \geqslant 1$.

The functions m are the moments which correspond to the cumulants appearing in the exponent on the lhs of Eq. (47). So the nth moment m_n contains cumulants up to the nth. Thus the rhs of Eq. (48) contains h_ks from $k = 1$ to $k = n - 1$, for example;

$$m_0 = 1, \quad m_1 = \epsilon s + h_1\,, \quad m_2 = m_1^2 + h_2\,, \quad m_3 = -2m_1^3 + 3m_1 m_2 + h_3\,, \text{ etc.} \tag{49}$$

This shows that the Ansatz for the solution of Eq. (48),

$$q_n(t) = \epsilon^{n-1} q_{n0}(t) + \epsilon^n q_{n1}(t) + \epsilon^{n+1} q_{n2}(t) + \cdots \tag{50}$$

is consistent. With this Ansatz, Eq. (46) gives

$$h_n = \epsilon^n h_{n0} + \epsilon^{n+1} h_{n1} + \cdots \tag{51}$$

where

$$\begin{aligned} h_{n0} &= -i\eta q_{n+1,0} \\ h_{n1} &= -i\eta q_{n+1,1} - \tfrac{1}{2}\eta^2 q_{n+2,0} \\ &\vdots \\ h_{n,k} &= \sum_{j=0}^{k} [1/(j+1)!](-i\eta)^{j+1}\, q_{n+1+j,k-j} \end{aligned} \tag{52}$$

and so the moments m_n have the expansions

$$m_n = \epsilon^n m_{n0} + \epsilon^{n+1} m_{n1} + \cdots \tag{53}$$

as is seen from Eq. (49). Thus both sides of Eq. (48) start from $O(\epsilon^{n-1})$, showing the consistency of the Ansatz (50).

This Ansatz gives to the characteristic function $Q(\xi, t)$ the following form:

$$Q(\xi, t) = \exp[(1/\epsilon)\, \psi(i\epsilon\xi, \epsilon, t)] \tag{54}$$

with

$$\psi(u, \epsilon, t) = \psi_0(u, t) + \epsilon\psi_1(u, t) + \epsilon^2\psi_2(u, t) + \cdots \tag{55}$$

where

$$\psi_k(u, t) = \sum_{n=1}^{\infty} (u^n/n!)\, q_{nk}(t) \tag{56}$$

This almost completes our proof. If the characteristic function $Q(\xi, t)$ has the form (54) at an initial time t_0, the expansion coefficients $q_{nk}(t)$ are determined for later times by Eq. (48) so that the same form (54) persists for $t > t_0$. In order to obtain the asymptotic form (35), we perform the inverse transform of (36),

$$\begin{aligned} P(x, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} Q(\xi, t) \exp(-i\xi x)\, d\xi \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\left[\frac{1}{\epsilon}\, \psi(i\epsilon\xi, \epsilon, t) - i\xi x\right] d\xi \end{aligned} \tag{57}$$

This can be evaluated by the method of steepest descent. Writing

$$i\epsilon\xi = u$$

the col of the function in the exponent in the integrand is determined by

$$\sum_{k=0}^{\infty} \epsilon^k (\partial/\partial u)\, \psi_k(u, t) = x \tag{58}$$

which gives the solution $u(x, t)$ in the form

$$u(x, t) = \sum_{k=0}^{\infty} \epsilon^k u_k(x, t) \tag{59}$$

Then Eq. (57) becomes

$$P(x, t) \simeq \left[2\pi \sum \epsilon^{k+1} \frac{\partial^2 \psi_k}{\partial u^2}\right]^{-1/2} \exp\left[\frac{1}{\epsilon} \phi(x, \epsilon, t) + O(\epsilon^2)\right] \tag{60}$$

where

$$\phi(x, \epsilon, t) = \left[\sum \epsilon^k \psi_k(u, t) - ux\right]_{u=u(x,t)} \tag{61}$$

which is written as

$$\phi(x, t) = \sum_{k\geqslant 0} \epsilon^k \phi_k(x, t) \tag{62}$$

namely as an asymptotic expansion for small ϵ or large Ω.

Thus the asymptotic form of $P(x, t)$, (35), or more precisely (60), which we call the extensive property of $P(x, t)$, indeed propagates in time; if it is valid at an initial time, it will remain so at later times. It should be noted, however, that this assertion may break down if the convergence properties implicitly assumed in the above arguments are lost at a certain time. This may be relevant in critical regions.

If the distribution of x is the delta function

$$P(x, t_0) = \delta(x - x_0)$$

at the initial time t_0, the initial characteristic function is simply

$$Q(\xi, t) = e^{i\xi x_0}$$

so that

$$\psi(u, t_0) = ux_0 \tag{63}$$

is the initial condition for $\psi(u, \epsilon, t)$ of Eq. (55). Since this bears the extensive property, the transition probability $P(x, t \mid x_0, t_0)$ from x_0 to x in a time interval $(t_0 < t)$ is extensive and is expressed as

$$P(x, t \mid x_0, t_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\left[\frac{1}{\epsilon} \psi(i\epsilon\xi, t \mid x_0, t_0) - i\xi x\right] d\xi \tag{64}$$

where $\psi(u, t \mid x_0, t_0)$ is the function (55) determined by the initial condition (63). Asymptotic evaluation of this integral gives the expression

$$P(x, t \mid x_0, t_0) = [2\pi\Delta(x, t \mid x_0, t_0)]^{-1/2} \exp\left[\frac{1}{\epsilon}\phi(x, t \mid x_0, t_0)\right] \tag{65}$$

for the transition probability, where Δ is a quantity of $O(\epsilon)$. The function $\phi(x, t \mid x_0, t_0)$ characterizes the extensive property of transition in a large system. For a path of transitions $(x_1, t_1; x_2, t_2; \ldots; x_n, t_n)$ we have the probability

$$P(x_1, t_1; x_2, t_2; \ldots; x_n, t_n) = \prod_{j=2}^{n} [2\pi\Delta(x_j, t_j \mid x_{j-1}, t_{j-1})]^{-1/2} \exp\left[\frac{1}{\epsilon}\sum_{j=2}^{n}\phi(x_j, t_j \mid x_{j-1}, t_{j-1})\right] \tag{66}$$

The leading terms in $\psi(\xi, \epsilon, t)$ in (56) are easily determined by Eq. (48). To the order of ϵ^0, this gives

$$\dot{q}_{10}(t) = (1/2\pi)\int d\eta \int dr\, r\, w[\eta, r, t]\, e^{-iq_{10}\eta} \tag{67}$$

Inserting (38) into the integrand, we have

$$\dot{q}_{10}(t) = c_1(q_{10}, t) \tag{68}$$

where c_1 is the first moment of transition, or the average velocity, defined by Eq. (14). To the order of ϵ we have from Eqs. (48), (49), and (52)

$$\tfrac{1}{2}\dot{q}_{20}(t) = \tfrac{1}{2}c_2(q_{10}) + (\partial c_1(q_{10})/\partial q_{10})\, q_{20} \tag{69}$$

In like manner we have

$$\frac{1}{3}\dot{q}_{30}(t) = \frac{1}{3}c_3(q_{10}) + \frac{\partial c_2(q_{10})}{\partial q_{10}} q_{20} + \frac{\partial^2 c_1(q_{10})}{\partial q_{10}^2} q_{20}^2 + \frac{\partial c_1(q_{12})}{\partial q_{10}} q_{30} \tag{70}$$

to determine $q_{30}(t)$ and similar but more complicated equations for higher $q_{n0}(t)$. The temperal evolution of $q_{n0}(t)$ is governed by that of lower order q_{n0} and the moments of transition up to the nth. The function ψ_0 in Eq. (55) is constructed in this way.

The higher-order functions ψ_1, etc., in Eq. (55) are also obtained in a successive way. For example, $q_{11}(t)$ follows the equation

$$\dot{q}_{11}(t) = c_1'(q_{10})\, q_{11} + \tfrac{1}{2}c_1''(q_{10})\, q_{20} \tag{71}$$

The evolution of $q_{21}(t)$ is determined by that of q_{10}, q_{20}, q_{11}, and q_{30}. Thus

Eq. (48) suffices to determine the evolution of the cumulant function $\psi(\xi, \epsilon, t)$ in (54).

By definition, q_{10}, q_{11}, and q_{20} correspond to the average and the variance of x, to the order of ϵ. We write for convenience

$$\langle x_t \rangle = y(t) + \epsilon u(t) + O(\epsilon^2), \qquad y(t) \equiv q_{10}(t), \qquad u(t) = q_{11}(t) \tag{72}$$

and

$$\langle [x_t - \langle x_t \rangle]^2 \rangle = \epsilon\sigma(t) + O(\epsilon^2), \qquad \sigma(t) \equiv q_{20}(t) \tag{73}$$

The Gaussian approximation for $P(x, t)$ is thus simply given by

$$P(x, t) = (2\pi\epsilon\sigma)^{-1/2} \exp\left[-\frac{1}{2\epsilon\sigma(t)}[x - y(t) - \epsilon u(t)]^2\right] \tag{74}$$

For the multigate transition probability (66) the Gaussian approximation is given by

$$\begin{aligned} &P(x_1, t_1 ; x_2, t_2 ;\ldots; x_n, t_n) \\ &\quad = \prod_{j=2}^{n} [2\pi\epsilon\sigma(t_j \mid x_{j-1}, t_{j-1})]^{-1/2} \\ &\qquad \times \exp - \sum \frac{[x_j - y(t_j \mid x_{j-1}, t_{j-1}) - \epsilon u(t_j \mid x_{j-1}, t_{j-1})]^2}{2\epsilon\sigma(t_j \mid x_{j-1}, t_{j-1})} \end{aligned} \tag{75}$$

where $y(t \mid x', t')$, $\sigma(t \mid x', t')$, and $u(t \mid x', t')$ are solutions of Eqs. (68), (69), and (71) with the initial conditions

$$y(t') = x', \qquad \sigma(t') = 0, \qquad u(t') = 0. \tag{76}$$

With or without the correction ϵu in the exponent, the transition probability (75) satisfies the Markovian property

$$\int P(x_1, t_1 ; x', t')\, dx'\, P(x', t' ; x_2, t_2) = P(x_1, t_1 ; x_2, t_2)$$

This is confirmed with the use of Eqs. (69) and (71) or of Eq. (95). The transition probability (75) describes the processes $x(t)$ in a Gaussian approximation. This will be discussed in later sections.

4. EVOLUTION EQUATIONS

We have seen that the cumulant function ψ in Eq. (54) is determined by a set of evolution equations like (68)–(70). These equations can be more

directly obtained from the Ansatz (35). This has been shown already by Kubo[4] but here we discuss this matter in a little more detail.

Let us assume that the probability $P(x, t)$ has the extensive property so that it is written as

$$P(x, t) = C \exp[(1/\epsilon)\, \phi_0(x, t) + \phi_1(x, t) + O(\epsilon)] \tag{77}$$

The normalization factor in Eq. (60) contains functions of x and t in successive powers of ϵ, but they can be conveniently absorbed into the exponent of the expression (77), so that the factor C is a constant of order $\epsilon^{-1/2}$. Inserting (77) into Eq. (12), we get

$$\frac{\partial}{\partial t}\, \phi_0(x, t) = -\int dr\, w(x, r)\Big[1 - \exp\Big(-r\, \frac{\partial \phi_0}{\partial x}\Big)\Big] \tag{78}$$

and

$$\frac{\partial}{\partial t}\, \phi_1(x, t) = \int dr\, \Big[w(x, r)\Big(\frac{1}{2}\, r^2\, \frac{\partial^2 \phi_0}{\partial x^2} - r\, \frac{\partial \phi_1}{\partial x}\Big) - r\, \frac{\partial w}{\partial x}\Big] \exp\Big(-r\, \frac{\partial \phi_0}{\partial x}\Big) \tag{79}$$

to determine ϕ_0 and ϕ_1.

The Gaussian approximation (73) suggests a method to solve Eq. (78). We put

$$x = y(t) + z \tag{80}$$

and

$$\phi_0(x, t) = g_0(z, t) \tag{81}$$

in Eq. (78), which is then written as

$$\frac{\partial}{\partial t}\, g_0(z, t) - \dot{y}(t)\, \frac{\partial}{\partial z}\, g_0(z, t) = -\int w(y + z, r)\, dr\, \Big[1 - \exp\Big(-r\, \frac{\partial g_0}{\partial z}\Big)\Big] \tag{82}$$

and choose $y(t)$ so as to satisfy the equation

$$\dot{y}(t) = c_1(y) \tag{83}$$

This makes the terms linear in $\partial g_0/\partial z$ vanish from the equation. Inserting (80) and (83) into (82) and expanding in powers of z by assuming the solution

$$g_0(z, t) = a_2(t)\, z^2 + a_3(t)\, z^3 + \cdots \tag{84}$$

we obtain a set of ordinary differential equations, which we call the evolution

equations, for the expansion coefficients. The first few members of these equations are

$$\dot{a}_2(t) = 2c_2(y)\, a_2^2 - 2c_1'(y)\, a_2 \tag{85}$$

$$\dot{a}_3(t) = 6c_2(y)\, a_2 a_3 - \tfrac{4}{3}c_3(y)\, a_2^3 - 3c_1(y)\, a_3 + 2c_2'(y)\, a_2^2 - c_1'(y)\, a_2 \tag{86}$$

If we put

$$a_2 = -[2\sigma(t)]^{-1} \tag{87}$$

Eq. (85) becomes

$$\dot{\sigma}(t) = 2c_1'(y)\, \sigma(t) + c_2(y) \tag{88}$$

reproducing (69). Equations for higher-order coefficients in expression (84) and those in the similar expansion of ϕ_1 can be derived in the same way. Thus the function g_0 in Eq. (81) gives the Gaussian approximation (73) in the second order of z, but the above method yields a more complete expression for $\phi_0(x, t)$ including higher orders of z.

This calculation can easily be generalized to a vector variable $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ representing a set of macrovariables. Clearly Eq. (83) now reads

$$\dot{y}_j(t) = c_{1j}(\mathbf{y}) \tag{89}$$

where

$$c_{1j}(\mathbf{y}) = \int dr\, r_j w(y_1, \ldots, y_n, r_1, \ldots, r_n) \tag{90}$$

are the average velocity. Equation (88) takes the somewhat complicated form

$$\dot{\sigma}_{jk}(t) = \sum_l \left(\sigma_{jl} \frac{\partial c_{1k}}{\partial y_l} + \frac{\partial c_{1j}}{\partial y_l} \sigma_{lk}\right) + c_{2jk} \tag{91}$$

where

$$c_{2jk}(\mathbf{y}) = \int dr\, r_j r_k w(y_1, \ldots, y_n, r_1, \ldots, r_n) \tag{92}$$

are the second moments of transition. The distribution function $P(x, t)$ is written as

$$P(x, t) = C \exp\left\{-\frac{1}{2\epsilon} \sum \sigma_{jk}^{-1}[x_j - y_j(t)][x_k - y_k(t)] + \cdots\right\} \tag{93}$$

in the Gaussian approximation, where σ^{-1} is the inverse matrix of the variance matrix σ.

The variance matrix σ evolves in time following Eq. (91). It is governed by the first and second moments of transition which vary in time according

to the evolution of the average (or the most probable) motion $y(t)$ of x as determined by Eq. (89). In the special case of a single variable the variance $\sigma(t)$ is determined by the value of y at that instant provided that the transition probability w does not explicitly depend on time. Then Eq. (88) is written as

$$c_1(y)\frac{d\sigma}{dy} = 2\frac{dc_1}{dy}\sigma + c_2(y) \tag{94}$$

with the use of Eq. (83). This equation is easily integrated to give

$$\sigma(y) = \sigma_0\left[\frac{c_1(y)}{c_1(y_0)}\right]^2 + c_1^2(y)\int_{y_0}^{y}\frac{c_2(y')\,dy'}{c_1(y')^3} \tag{95}$$

with the initial conditions

$$y = y_0\,, \qquad \sigma = \sigma_0 \qquad \text{at} \quad t = t_0$$

Later we shall discuss some implications of this equation.

Here it may be worthwhile to comment on van Kampen's method in connection with the method developed in this section. Van Kampen[1] pointed out quite rightly that the Kramers–Moyal equation (13) is not by itself a systematic way of expanding in the smallness parameter ϵ. For example, if it is terminated at the second term of the rhs of (13),

$$\frac{\partial}{\partial t}P(x,t) = -\frac{\partial}{\partial x}c_1(x,t)\,P(x,t) + \frac{\epsilon}{2}\frac{\partial^2}{\partial x^2}c_2(x,t)\,P(x,t) \tag{96}$$

it looks like a Fokker–Planck equation, which, however, requires great caution to handle. In the case when the coefficients c_1 and c_2 do not explicitly depend on time Eq. (96) does not reproduce a correct equilibrium solution. It gives only the Gaussian approximation as given by Eq. (3) if the stationary solution is expanded around the maximum. This is all right, but an honest solution of Eq. (96) is generally meaningless except under the simple situation where c_1 is linear in x and c_2 is constant. In other words, as van Kampen has emphasized, a Fokker–Planck equation containing a nonlinear function $c_1(x)$ is at least a very tricky object.

This means that the use of a Fokker–Planck equation of the type (96) should be looked out for when a nonlinear relaxation process is under consideration. At the same time it should be remembered that the generally accepted equation

$$\frac{\partial}{\partial t}P(x,t) = \frac{\partial}{\partial x}D(x)\left(\frac{\partial F_e}{\partial x} + \frac{1}{kT}\frac{\partial}{\partial x}\right)P(x,t) \tag{97}$$

is hardly justified as a genral equation. This equation is of course correct if the equilibrium free energy $F_e(x)$ is quadratic in x. There is no general validity, however, unless it is actually derived from a more basic microscopic calculation. A simple counterexample will suffice to illustrate this. In Eq. (15) if the molecular field constant α is zero, the model is for noninteracting Ising spins, for which c_1 is linear in x as is seen by Eq. (20). Relaxation of the spins follows a simple exponential decay. On the other hand, the "thermodynamic force" derived from the free energy is nonlinear and so Eq. (97) will not reproduce simple relaxation of spins unless a very artificial assumption is made for the diffusion coefficient D in (97).

As a systematic method of expansion van Kampen used the following method. In the Kramers–Moyal equation he put

$$x = y(t) + \epsilon^{1/2}\xi \tag{98}$$

choosing $y(t)$ so as to satisfy Eq. (83). Then Eq. (13) is transformed into the equation

$$\frac{\partial}{\partial t}\bar{P}(\xi, t) = -\epsilon^{-1/2}\frac{\partial}{\partial \xi}[c_1(y + \epsilon^{1/2}\xi) - c_1(y)]\,\bar{P}(\xi, t) + \sum_{n=2}^{\infty}(-)^n \frac{\epsilon^{(n-2)/2}}{n!}\left(\frac{\partial}{\partial \xi}\right)^n c_n(y + \epsilon^{1/2}\xi)\,\bar{P}(\xi, t) \tag{99}$$

for the function

$$\bar{P}(\xi, t) = P(x, t)$$

In the limit of $\epsilon \to 0$, Eq. (99) reduces to

$$\frac{\partial}{\partial t}\bar{P}(\xi, t) = -\frac{\partial}{\partial \xi}c_1'(y)\,\xi\bar{P} + \frac{1}{2}\frac{\partial^2}{\partial \xi^2}c_2(y)\,\bar{P} \tag{100}$$

which is a Fokker–Planck equation with time-dependent coefficients $c_1(y)$ and $c_2(y)$. It is easily confirmed that the Gaussian distribution (73) with $y(t)$ and $\sigma(t)$ determined by Eqs. (83) and (88) is in fact the solution of Eq. (100) for given initial conditions. It is thus seen that the Fokker–Planck equation (96) should not be solved too honestly but only with the Ansatz (98) in order to give a meaningful result.

If one proceeds from the Gaussian approximation to higher approximations, one obtains a function which is a solution in the form of (62). In order to determine the function

$$\begin{aligned}(1/\epsilon)\,\phi_0(x, t) &= \bar{\phi}(\xi, t) \\ &= a_2(t)\,\xi^2 + \epsilon^{1/2}a_3(t)\,\xi^3 + \epsilon a_4(t)\,\xi^4 + \cdots\end{aligned} \tag{101}$$

for example, all orders of the expansion (99) have to be considered. This procedure is tedious and unpractical. One can reach instead the same result more directly by using $g_0(z, t)$, (81), which is obtained from Eq. (82). As we have seen already, the Ansatz (77) and the transformed equations (78) and (79) and the like provide us with a convenient means to attain an asymptotic solution with the entensive property.

It is also possible to express $P(x, t)$ in Eq. (12) by a path integral and to formulate the problem through variational principle and the associated Hamilton–Jacobi equations. This approach is briefly sketched in the appendices.

5. NORMAL FLUCTUATION, RELAXATION, AND RESPONSE NEAR EQUILIBRIUM

We consider some consequences of the evolution equations

$$\dot{y}(t) = c_1(y) \tag{102}$$

$$\dot{\sigma}(t) = 2c_1'(y)\,\sigma + c_2(y) \tag{103}$$

$$\dot{u}(t) = c_1'(y)\,u + \tfrac{1}{2}c_1''(y)\,\sigma \tag{104}$$

which were derived in the preceding sections [Eqs. (68), (69), (71), (83), (88)]. The first equation determines the most probable path of $x(t)$, to $O(\epsilon^0)$, which may be called the *deterministic motion* of x. The second equation gives the variance σ of $x(t)$ at time t(for brevity σ is called hereafter the variance although by usual definition the variance is $\epsilon\sigma$). The third equation gives, to $O(\epsilon)$, the deviation of the average from the deterministic path which comes from the nonlinearity of $c_1(y)$. In the case of a single variable, σ and u can be given as functions of y [cf. Eq. (95)].

The simplest example is classical Brownian motion, for which we put

$$c_1(y) = -\gamma y, \qquad c_2(y) = \text{const} = c \tag{105}$$

Equation (102) then gives a simple relaxation,

$$\dot{y} = -\gamma y, \qquad y(t) = y_0 e^{-\gamma t}$$

and Eq. (103) the variance

$$\begin{aligned}\sigma(y) &= \frac{c}{2\gamma} + \left(\sigma_0 - \frac{c}{2\gamma}\right)\left(\frac{y}{y_0}\right)^2 \\ &= \sigma_e + (\sigma_0 - \sigma_e)\, e^{-2\gamma t}\end{aligned} \tag{106}$$

where

$$\sigma_e = c/2\gamma \tag{107}$$

is the variance in equilibrium $y = 0$. This is directly obtained from Eq. (103) as the stationary solution of σ. The equilibrium distribution of x is

$$P_e(x) = (2\pi\epsilon\sigma_e)^{-1/2} \exp(-x^2/2\epsilon\sigma_e) \tag{108}$$

and the nonequilibrium distribution is

$$P(x, t) = [2\pi\epsilon\sigma(t)]^{-1/2} \exp\left[-\frac{1}{2\epsilon\sigma(t)}(x - y_0 e^{-\gamma t})^2\right] \tag{109}$$

if the initial distribution is

$$P(x, 0) = (2\pi\epsilon\sigma_0)^{-1/2} \exp\left[-\frac{1}{2\epsilon\sigma_0}(x - y_0)^2\right] \tag{110}$$

This process is described by the standard Fokker–Planck equation,

$$\frac{\partial}{\partial t} P(x, t) = \frac{\partial}{\partial x}\left(\gamma x + \frac{1}{2}\epsilon c \frac{\partial}{\partial x}\right) P(x, t) \tag{111}$$

The general solution of this equation is a superposition of the solutions of (109) obtained by multiplying it by an arbitrary function of y_0 and integrating over y_0 (taking σ_0 to be zero). The autocorrelation of $x(t)$ is easily found to be

$$\langle x(t_1)\, x(t_2)\rangle = \langle x(t_1)^2\rangle \exp[-\gamma(t_2 - t_1)], \qquad t_1 < t_2 \tag{112}$$

This is in accordance with Doob's theorem: In a Gaussian Markovian process the autocorrelation decays by a simple exponential law. It should be remembered that this is essentially connected with the law of linear relaxation. This statement obviously applies more generally to a set of macrovariables. Namely, if Eq. (104) hold for a vector variable $\mathbf{y}$ with constant relaxation matrix γ and a constant matrix c_2, the process is a multidimensional Gaussian Markovian process described by a Fokker–Planck equation. Relaxation of the macrovariables is linear and the correlation matrix decays in exponentially time.

An equilibrium point x_e is defined by the condition

$$c_1(x_e) = 0 \tag{113}$$

Note that the term *equilibrium* is used here in a wide sense. It is not necessarily a thermodynamic or a static equilibrium, but it can be a steady state with a constant flow, for example, in the case when the variable x is a current.

Around an equilibrium point x

$$\Delta\dot{y} = -\gamma_e \Delta y + O(\Delta y) \tag{114}$$

if

$$\gamma_e = -\left.\frac{\partial c_1(x)}{\partial x}\right|_{x=x_e} \tag{115}$$

is not zero. If γ_e is zero, we call it a marginal equilibrium, which will be treated in a later section. If $\gamma_e < 0$, the equilibrium is unstable; the system will depart from x_e when an infinitesimal deviation determines the direction of departure.

In a stable equilibrium, $\gamma_e > 0$, the probability distribution of deviation

$$\Delta x = x - x_e$$

from the stable point x_e is given by a Gaussian distribution,

$$P(\Delta x) = (2\pi\epsilon\sigma_e)^{-1/2} \exp\left\{-\frac{1}{\epsilon}\left[\frac{(\Delta x)^2}{2\sigma_e} + O(\epsilon)\right]\right\} \tag{116}$$

with the variance σ_e given by a stationary solution of Eq. (103), namely

$$\sigma_e = -\tfrac{1}{2}c_2(x_e)/c_1'(x_e) = \tfrac{1}{2}c_2(x_e)/\gamma_e \tag{117}$$

If the transition probabilities are defined by Eq. (30), we have, from Eqs. (33) and (34)

$$c_1'(x) = -\gamma_e \Delta x + O(\Delta x^3), \qquad c_2(x) = 2\gamma_e/\beta f_e''(x_e) + O(\Delta x^2) \tag{118}$$

where

$$\gamma_e = \beta f_e''(x_e) \int_{r>0} dr\, r^2 \bar{w}_0(x_e, r) \tag{119}$$

This gives

$$\sigma_e^{-1} = \beta f_e''(x_e) \tag{120}$$

in accordance with the distribution (3).

Spontaneous fluctuations around x_e are normally very small, of the order of $\epsilon^{1/2}$. So the Kramers–Moyal equation (13) simply reduces to the Fokker–Planck equation (111) with $\gamma = \gamma_e$ and $c = c_2(x_e)$. Fluctuations are the standard Brownian noise. The correlation function of spontaneous fluctuations thus decays exponentially following (112). The macrovariable Δy relaxes in the same way even when its magnitude is much larger than that

of the fluctuations. Namely the linear law of relaxation holds for Δy to $O(\epsilon^0)$ as long as

$$|\Delta y| \ll \gamma_e / \tfrac{1}{2} c_1''(x_e)$$

This almost trivial fact is noted here in connection with Onsager's old assumption which asserts that the average regression of spontaneous fluctuations near equilibrium is governed by the relaxation law of the corresponding macrovariable. In the framework of our present approach this statement holds for a thermodynamic equilibrium as well as a nonthermodynamic steady state as long as the equilibrium is stable and nonmarginal.

When the system is subjected to an external force K the equilibrium is shifted by the force. The effect of such an external force is incorporated in the evolution equations in the following two typical ways.

(a) The force simply modifies the drift velocity as

$$c_1(x, K) = c_1(x) + K \tag{121}$$

and leaves other c_n unaltered. This means that the force drives the system by

$$\dot{y} = c_1(y) + K \tag{122}$$

A shifted equilibrium is determined by

$$c_1(x_K) + K = 0 \tag{123}$$

Variations around the equilibrium x_K are described, in a linear range, by

$$\Delta \dot{y} = -\gamma_K \Delta y + \Delta K, \qquad \gamma_K = -(\partial/\partial x_K)\, c_1(x_K) \tag{124}$$

(b) The external force modifies the equilibrium free energy f_e in Eq. (29), or more generally the function ϕ_e in Eq. (1). If the free energy exists, it is generally changed into

$$c_1(x, K) = -2 \int dr\, r \bar{w}_K(x, r) \sinh \left[\frac{\beta}{2} r \left(\frac{\partial f_e}{\partial x} - K \right) \right] \tag{125}$$

$$c_2(x, K) = 2 \int dr\, r^2 \bar{w}_K(x, r) \cosh \left[\frac{\beta}{2} r \left(\frac{\partial f_e}{\partial x} - K \right) \right] \tag{126}$$

where the symmetrized transition probability $\bar{w}$ may depend on K as indicated by the subscript K. A stable equilibrium x_K under the force K is determined by

$$f_e'(x_K) = K \tag{127}$$

Around the equilibrium, variations in linear ranges follow the equation

$$\Delta\dot{y} = -\gamma_K(\Delta y - \chi_K \Delta K) \tag{128}$$

Noticing that

$$-\frac{1}{f_e''(x_K)}\frac{\partial c_1(x_K, K)}{\partial x_K} = \frac{\partial c_1(x_K, K)}{\partial K} = \frac{\beta}{2} c_2(x_K, K) \tag{129}$$

as obtained from Eqs. (126) and (127), we find that

$$\gamma_K = -\frac{\partial c_1(x_K, K)}{\partial x_K} = \frac{1}{2}\beta f_e''(x_K)\, c_2(x_K, K) \tag{130}$$

and

$$\chi_K = \frac{1}{\gamma_K}\frac{\partial c_1(x_K, K)}{\partial K} = \frac{\beta}{2\gamma_K} c_2(x_K, K) \tag{131}$$

Spontaneous fluctuations around x_K in the absence of ΔK are normal Brownian fluctuations. In accord with the linear equations (124) and (128) with $\Delta K = 0$, the autocorrelation of the fluctuation $\Delta x = x - x_K$ behaves normally as

$$\langle \Delta x(t_1)\, \Delta x(t_2)\rangle = \epsilon\sigma_K e^{-\gamma_K(t_1 - t_2)} \tag{132}$$

where the equilibrium variance σ_K is given by

$$\langle \Delta x^2\rangle = \epsilon\sigma_K = \tfrac{1}{2}\epsilon c_2(x_K, K)/\gamma_K \tag{133}$$

This shows that the differential admittance $\mu(\omega)$ is expressed as

$$\mu_K(\omega) = \frac{1}{i\omega + \gamma_K} = \frac{1}{\epsilon\sigma_K}\int_0^\infty \langle \Delta x(t_0)\, \Delta x(t_0 + t)\rangle\, e^{-i\omega t}\, dt \tag{134}$$

in case (a) and as

$$\begin{aligned}\chi_K(\omega) &= \frac{1}{i\omega + \gamma_K}\gamma_K\chi_K(0) \\ &= \frac{\beta}{\epsilon}\left[\langle \Delta x^2\rangle - i\omega\int_0^\infty \langle \Delta x(t_0)\, \Delta x(t_0 + t)\rangle\, e^{-i\omega t}\, dt\right]\end{aligned} \tag{135}$$

in case (b). This is the fluctuation-dissipation theorem[7] for the differential admittance around a shifted equilibrium and the spontaneous fluctuation spectrum.

6. FLUCTUATIONS IN STATES FAR FROM EQUILIBRIUM

As long as a system never passes through a marginal, critical, or unstable equilibrium point in the course of its evolution, fluctuations of the macrovariable around the deterministic path can be described as a Gaussian process as was noted in Section 3. It is important to notice that the multigate transition probability (75) can be expressed as a path integral,

$$P(x_1, t_1; x_2, t_2; \ldots; x_n, t_n) = \int \mathcal{D} \exp\left\{-\int_{t_1}^{t_n} \frac{1}{2\epsilon c_2(x_t)} \left[\frac{dx_t}{dt} - c_1(x_t)\right]^2 dt\right\} \tag{136}$$

where x_t is a path starting from x_1 at time t_1, passing x_2 at t_2,..., and ending at x_n at t_n. The integral over the paths is carried out with a properly defined measure of paths similar to the case of a Wiener integral or of a Feynman integral. In order to see this, we simply note that Eqs. (102)–(104) are integrated over a short time interval Δt to give

$$\begin{aligned} y(t + \Delta t \mid x_t, t) &= x_t + c(x_t)\,\Delta t + O(\Delta t^2) \\ \sigma(t + \Delta t \mid x_t, t) &= c_2(x_t)\,\Delta t + O(\Delta t^2) \\ u(t + \Delta t \mid x_t, t) &= O(\Delta t^2) \end{aligned}$$

Thus the expression in the exponent in Eq. (75) becomes

$$\begin{aligned} &\frac{1}{2\epsilon} \sum \left\{\frac{1}{2c_2(x_t)\,\Delta t} [x_{t+\Delta t} - x_t - c_1(x_t)\,\Delta t]^2 + O(\Delta t^2)\right\} \\ &\quad = \frac{1}{2\epsilon} \sum \frac{1}{2c_2(x_t)} \left[\frac{dx_t}{dt} - c_1(x_t)\right]^2 \Delta t + O(\Delta t^2) \end{aligned}$$

if the successive time intervals are all equal to Δt. Taking the limit of $\Delta t \to 0$ and keeping fixed points $x_1, x_2, \ldots, x_n$ at $t_1, t_2, \ldots, t_n$ the summation over all possible intermediate points goes over to the path integral (136). An explicit integration over paths is usually rather hard, but one can convince himself easily that Eq. (136) gives, for example, the result (109) by elementary calculations. A more general formulation of the path integral solution of Eq. (10) is given in Appendix A.

Now we consider a deterministic path $(y_0, t_0) \to (y_1, t_1)$. Around this path each realization x_t may occur as a fluctuation with the probability proportional to the integrand of the expression (136). This can be described in the Gaussian approximation by the evolution of the parameters y_t, σ_t, and u_t as determined by Eqs. (102)–(104) with the initial conditions

$$y = y_0, \qquad \sigma = \sigma_0, \qquad u = u_0 = 0$$

at t_0. The correlation function of fluctuations is defined by

$$\begin{aligned}\langle \Delta x_\tau \, \Delta x_t \rangle &= \langle x_\tau x_t \rangle - \langle x_\tau \rangle \langle x_t \rangle \\ &= \langle x_\tau x_t \rangle - y_\tau y_t - \epsilon u_\tau y_t - \epsilon y_\tau u_t + O(\epsilon^2)\end{aligned} \tag{137}$$

for $t_0 < \tau < t < t_1$ since we have $\langle x_t \rangle = y_t + \epsilon u_t$. The expression (137) is a quantity of order ϵ. For the whole system the corresponding quantity is the correlation

$$\langle \Delta X_\tau \, \Delta X_t \rangle = \Omega \langle \Delta x_\tau \, \Delta x_t \rangle$$

which is proportional to the size, as is actually observed by experiments.

By definition we have

$$\langle x_\tau x_t \rangle = \int dx_\tau \int dx \, x_\tau P(x_\tau , \tau) \, P(x_\tau , \tau; x, t) \, x \tag{138}$$

which is found to be

$$\langle x_\tau x_t \rangle = \langle x_\tau y(t \mid x_\tau , \tau) \rangle + \epsilon \langle x_\tau u(t \mid x_\tau , \tau) \rangle \tag{139}$$

with the use of Eq. (75). The average here is taken over the distribution $P(x_\tau , \tau)$. Considering the Gaussian distribution of x_τ around the average $y_\tau + \epsilon u_\tau$ with the variance equal to $\epsilon \sigma_\tau$, we expand the first term on the rhs of Eq. (139), to first order in ϵ, as

$$\begin{aligned}&\langle (\langle x_\tau \rangle + \Delta x_\tau) \, y(t \mid \langle x_\tau \rangle + \Delta x_\tau , \tau) \rangle \\ &\quad = \langle x_\tau \rangle \, y(t \mid \langle x_\tau \rangle, \tau) + \epsilon \sigma_\tau (\partial / \partial \langle x_\tau \rangle) \, y(t \mid \langle x_\tau \rangle, \tau) \\ &\qquad + \tfrac{1}{2} \epsilon \sigma_\tau \langle x_\tau \rangle (\partial^2 / \partial \langle x_\tau \rangle^2) \, y(t \mid \langle x_\tau \rangle, \tau) + O(\epsilon^2)\end{aligned} \tag{140}$$

The first term of the above expression is again expanded in ϵ as

$$\langle x_\tau \rangle \, y(t \mid \langle x_\tau \rangle, \tau) = y_\tau y_t + \epsilon u_\tau y_t + \epsilon y_\tau u_\tau (\partial y_t / \partial y_\tau) + O(\epsilon^2)$$

In the second term of the rhs of Eq. (139) x_τ can be replaced by y_τ. Thus we have from Eqs. (138)–(140)

$$\langle \Delta x_\tau \, \Delta x_t \rangle = \epsilon y_\tau \left[-u_t + u(t \mid y_\tau , \tau) + u_\tau \frac{\partial y_t}{\partial y_\tau} + \frac{1}{2} \sigma_\tau \frac{\partial^2 y_t}{\partial y_\tau^2} \right] + \epsilon \sigma_\tau \frac{\partial y_t}{\partial y_\tau} \tag{141}$$

Note that $u(t \mid y_\tau , \tau)$ is not equal to u_t, because it is the solution of Eq. (104) with the initial conditions at time τ that $y = y_\tau$, $\sigma = 0$, and $u = 0$. The basic Markovian property, which is preserved in the Gaussian approximation (74), requires that the expression in the bracket on the rhs of Eq. (141) should

identically vanish. This can also be checked directly by explicit solution of Eqs. (102)–(104), namely

$$u_t(y_t) = u(t \mid y_0, t_0) = \tfrac{1}{2}c_1(y_t) \int_{y_0}^{y_t} [c_1''(y)/c_1(y)^2]\, \sigma_t(y)\, dy \tag{142}$$

$$u(t \mid y_\tau, \tau) = \tfrac{1}{2}c_1(y_t) \int_{y_0}^{y_t} [c_1''(y)/c_1(y)^2]\, \sigma'(y)\, dy \tag{143}$$

where

$$\sigma_t(y_t) = c_1(y_t)^2 \left[\int_{y_0}^{y_t} \frac{c_2(y)\, dy}{c_1(y)^3} + \frac{\sigma_0}{c_1(y_0)^2}\right] \tag{144}$$

$$\sigma'(y_t) = \sigma(t \mid y_\tau, \tau) = c_1(y_t)^2 \int_{y_\tau}^{y_t} \frac{c_2(y)\, dy}{c_1(y)^3} \tag{145}$$

and the relations

$$\partial y_t/\partial y_\tau = c_1(y_t)/c_1(y_\tau) \tag{146}$$

$$\partial^2 y_t/\partial y_\tau^2 = [c_1(y_t)/c_1(y_\tau)^2][c_1'(y_t) - c_1'(y_\tau)] \tag{147}$$

obtained from Eq. (102).

For a set of macrovariables $\mathbf{x} = (x_\alpha)$, Eq. (141) is generalized to the correlation matrix

$$\langle \Delta x_{\alpha\tau}\, \Delta x_{\beta t}\rangle = \epsilon y_{\alpha\tau} \left[-u_{\beta t} + u_{\gamma\tau} \frac{\partial y_{\beta t}}{\partial y_{\gamma\tau}} + \frac{1}{2}\, \sigma_{\gamma\delta\tau} \frac{\partial^2 y_{\beta t}}{\partial y_{\gamma\tau}\, \partial y_{\delta\tau}} + u_\beta(t \mid \mathbf{y}_\tau, \tau)\right] + \epsilon\sigma_{\alpha\gamma\tau} \frac{\partial y_{\beta t}}{\partial y_{\gamma\tau}} \tag{148}$$

where the usual convention is used for summation over dummy indices. The expression in the brackets on the rhs of the above equation vanishes as before because of the Markovian property.

So we arrive at the simple result

$$\langle \Delta x_{\alpha\tau}\, \Delta x_{\beta t}\rangle = \epsilon \sum_\gamma \sigma_{\alpha\gamma\tau}(\partial y_{\beta t}/\partial y_{\gamma\tau}) \tag{149}$$

or in the case of a single variable

$$\langle \Delta x_\tau \Delta x_t\rangle = \epsilon\sigma_\tau\, \partial y_t/\partial y_\tau \tag{150}$$

which is written as

$$\langle \Delta x_\tau \Delta x_t\rangle = \epsilon\sigma_\tau\, c_1(y_t)/c_1(y_\tau) \tag{151}$$

with the use of Eq. (149). Thus the correlation functions of fluctuations are

expressed in terms of the variance at time τ and the deterministic evolution of y in the interval (τ, t). A trivial example is a Brownian motion with a linear relaxation and a constant c_2, for which we have

$$\begin{aligned}\langle \Delta x_\tau \, \Delta x_t \rangle &= \epsilon \sigma_\tau y_t / y_\tau \\ &= \epsilon [\sigma_e + (\sigma_0 - \sigma_e) e^{-2\gamma\tau}] e^{-\gamma(t-\tau)}\end{aligned} \tag{152}$$

in accordance with Eq. (106).

For a nonlinear system the evolution of y and σ is more complex and is reflected in the more complicated behavior of the correlation function. Nonlinear effects in fluctuations show up when the system changes over a large range, for example, as relaxation from a state far from equilibrium, or as a forced process driven by a strong external perturbation. The above formulation provides us with a useful means to analyze such fluctuation or noise problems as acompany nonlinear processes, which have been treated by several authors, MacDonald and van Kampen, among others.[8] Applications of the present theory to such problems and the relationship of the present to previous theories will be discussed in a separate paper. Here we only remark that the above treatment suggests that nonlinear stochastic processes may be characterized by the functions $c_1(y)$ and $c_2(y)$ under normal situations. If these functions are known from a more basic theory or from experimental data, they can be used to predict the behavior of the system under general conditions. This approach seems to have wide applicability to a great variety of physical as well as nonphysical problems.

7. NONLINEAR RELAXATION AND ANOMALOUS FLUCTUATION NEAR UNSTABLE EQUILIBRIUM

If a system is near an unstable equilibrium, it will eventually depart toward a stable equilibrium. At the initial stage the macrovariable we observe will grow exponentially according to

$$\Delta \dot{y} \simeq \gamma' \, \Delta y \qquad \text{or} \qquad \Delta y \simeq \Delta y_0 \exp(\gamma' t) \tag{153}$$

where

$$\gamma' = c_1'(y_0) > 0$$

The fluctuation will also increase exponentially following Eq. (103) as

$$\sigma \simeq [\exp(2\gamma' t)] \Big[\sigma_0 + \int_0^t [\exp(-2\gamma'\tau)] \, c_2(y_\tau) \, d\tau \Big] \tag{154}$$

As the system approaches a new equilibrium the variance σ will reach a new

equilibrium, passing through a maximum. This is a general feature to be observed in a process of transition from an unstable to a stable equilibrium.

As a simple example we consider the case where

$$c_1(y) = (\gamma y/y_e)(y_e - y), \qquad c_2(y) = c_2 = \text{const} \tag{155}$$

The state $y = 0$ is an unstable equilibrium and the state $y = y_e$ is stable. For convenience we put

$$y = \tfrac{1}{2} y_e(1 - \cos\theta) \tag{156}$$

and assume that y is initially

$$0 < y = y_0 \ll y_e\,, \qquad \theta = \theta_0 \ll 1 \tag{151}$$

Then Eq. (95) gives

$$\sigma(y) = \sigma_0 \left(\frac{\sin\theta}{\sin\theta_0}\right)^4 + \sigma_e(\sin\theta)^4 \left\{\frac{\cos\theta_0}{\sin^4\theta_0} - \frac{\cos\theta}{\sin^4\theta} + \frac{3}{2}\left[\frac{\cos\theta_0}{\sin^2\theta_0} - \frac{\cos\theta}{\sin^2\theta}\right] + \frac{3}{8}\log\frac{\tan(\theta/2)}{\tan(\theta_0/2)}\right\} \tag{158}$$

where

$$\sigma_e = c_2/2\gamma$$

is the equilibrium value of σ at y_e, and σ_0 is the initial value at $y = y_0$. The variance (158) will attain a very large peak when the system is about half-way to the final equilibrium, namely when $y \sim y_e/2$. The height of the peak is approximately

$$\sigma_{\max} \simeq (\sigma_0 + \sigma_e)/(\sin\theta_0)^4 \tag{159}$$

which can be an enormous enhancement, for example, of 10^4 if $\theta_0 \sim 10^{-1}$.

Such a phenomenon may occur when a stable equilibrium is suddenly switched to an unstable state by a change of a certain parameter. Imagine, for example, a magnet which was initially above the Curie temperature suddenly cooled below the Curie temperature. Then a spontaneous magnetization eventually will develop. One would expect anomalous fluctuations to accompany such a change. By the sudden change of a certain condition a society may move toward a new equilibrium state, in the course of which movement an enormous uneasiness can be expected to arise. An example in physics seems to have been observed in laser phenomena, which has recieved a theoretical analysis[9] but not from such a general point of view as developed here.

If the system was initially at the exact unstable position, namely $\Delta y_0 = 0$

at $t = 0$ in Eq. (153), there will be no evolution of y for $t > 0$. However, the variance increases following Eq. (103), or

$$\dot{\sigma}(t) = 2\gamma'\sigma + c(y_0)$$

with an exponential growth to infinity. We can try for Eq. (78) a solution of the form

$$\phi_0(x, t) = (1/2\sigma)\, x^2 + b_1(t)\, x^3 + b_2(t)\, x^4 + \cdots$$

as a better approximation. But we find that $b_1(t)$, $b_2(t)$, etc., also approach zero with the passage of time. In a different representation, q_{30} in Eq. (70), q_{40}, etc., will be found to diverge because they have factors giving exponential growth. Thus the initial distribution, peaked at y_0, becomes flatter and flatter and after a latent time of the order of

$$\log \Omega/\gamma'$$

there will be a finite probability of finding the system at small but finite deviation, of the order of ϵ^0, out of the initial unstable position. Once such a deviation is realized, it will grow exponentially and approach a new equilibrium. A Gaussianlike distribution will evolve in this process to attain the final distribution. A precise description of this transition is, however, beyond the capacity of the approximation (74). We need a more careful analysis of Eq. (78) or of the basic equation (10). A Hamilton–Jacobi method can be used for this purpose, as is briefly described in Appendix B. More details will be given in a forthcoming paper.

Around an equilibrium point Eq. (102) may be assumed to have the expansion

$$\dot{y} = \gamma_1 y + \gamma_2 y^2 + \gamma_3 y^3 + \cdots \tag{160}$$

We can discriminate among different kinds of equilibrium by the following conditions:

(a) A stable equilibrium: $\gamma_1 < 0$.
(b) An unstable equilibrium: $\gamma_1 > 0$.
(c) A marginal equilibrium: $\gamma_1 = 0$ and $\gamma_2 \neq 0$.
(d) A critical equilibrium: $\gamma_1 = 0$, $\gamma_2 = 0$, $\gamma_3 \neq 0$.

There can be other cases depending on where the expansion starts, but the above cases are important. We have already discussed cases (a) and (b).

A well-known example of a critical equilibrium is a magnet at the Curie point. For the example of Weiss–Ising spins, as described by Eqs. (15)–(18), the critical point is given by

$$\alpha = \alpha_c = 1, \qquad \mu = 0 \tag{161}$$

In the neighborhood of this point the moments of transition are approximately

$$c_1 = 2[\mu + (\alpha - 1)\, y - (\tfrac{1}{2}\alpha^2 - \tfrac{1}{6}\alpha^3)\, y^3 + \cdots] \tag{162}$$

$$c = 2[1 + \tfrac{1}{2}(\alpha^2 - \alpha)\, y^2 + \cdots] \tag{163}$$

Clearly the paramagnetic state $y = 0$ is stable for $\mu = 0, \alpha < 1$. Ferromagnetic states appear for $\alpha > 1$. At zero magnetic field the spontaneous magnetization is given by the well-known equation

$$y_e = \tanh \alpha y_e \tag{164}$$

Equation (162) gives the approximation

$$y_e = \pm \left[\frac{\alpha - 1}{(\alpha^2/2) - (\alpha^3/6)}\right]^{1/2} \tag{165}$$

in the neighborhood of the critical point, which is the point where three equilibrium points, one unstable, two stable, coincide at $y = 0$. There Eq. (102) reads

$$\dot{y} = - \mid \gamma_3 \mid y^3 + \cdots \tag{166}$$

which means that a given deviation relaxes in time as

$$y = y_0/[1 + 2 \mid \gamma_3 \mid y_0^2 t]^{1/2} \tag{167}$$

This is a slow decay, which is related to the so-called critical slowingdown.

As is well known, the relationship between magnetization and the external magnetic field is represented by a hysteresis curve. When the magnetic field (or the parameter μ in our notation) is made to decrease from a large positive value, the magnetization y decreases from its saturation value. It remains positive until μ reaches a negative value, which we call μ_c, when a catastrophe occurs and the magnetization jumps to a negative value. This is seen from Eq. (102) with c_1 given by (20), but the essential points can be seen more easily by a simplified equation,

$$\dot{y} = \mu + ay - by^3 \equiv c_1(y, \mu) \tag{168}$$

which is suggested by Eq. (162). The function $c_1(y, \mu)$ has a maximum or a minimum at

$$y_\pm = \pm(a/3b)^{1/2}$$

As is shown in the Fig. 1, the c_1 curve touches the abscissa (at A) when the field μ is decreased to

$$\mu = -\mu_c = -2b(a/3b)^{3/2} \tag{169}$$

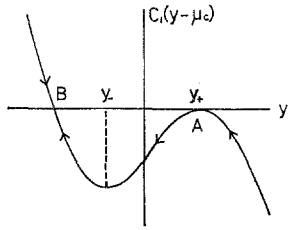

Fig. 1. A catastrophe

The point A is marginal. This is approached from the right ($y > y_+$). However, it is not stable because once this point is passed the final goal is B, which corresponds to the reversed magnetization. In the neighborhood of such a catastrophic point Eq. (102) has the form

$$\dot{y} = -\,|\,\gamma_2\,|\,y^2 + \cdots \tag{170}$$

(the origin of y is now placed at y_+). The relaxation follows the equation

$$y = y_0/(1 + y_0\,|\,\gamma_2\,|\,t) \tag{171}$$

which also describes the departure from y_0, if $y_0 < 0$, as long as

$$t \ll 1/|\,y_0\gamma_2\,|$$

This is again a sort of critical slowing down. The decay and the departure are slow and nothing like exponential. This is characteristic of a critical or a marginal point.

8. RELAXATION SPECTRA

If the process (7) is stationary in the sense that the transition probabilities W are independent of time, the stochastic operator on the rhs of Eq. (13), which we denote by Γ, is associated with the eigenvalue equation

$$\Gamma\Psi_\alpha \equiv -\sum \frac{(-)^n}{n!}\,\epsilon^{n-1}\left(\frac{\partial}{\partial x}\right)^n c_n(x)\,\Psi_\alpha = \lambda_\alpha\Psi_\alpha \tag{172}$$

If the operator Γ is such that it assures a unique equilibrium distribution $P_e(x)$, the eigenfunction

$$\Psi_0 = P_e$$

belongs to the eigenvalue $\lambda_0 = 0$. Other eigenfunctions may be called the relaxation modes because any solution of Eq. (7) or (13) can be expanded as

$$P(x, t) = P_e(x) + \sum_{\alpha \neq 0} b_\alpha \Psi_\alpha(x)\, e^{-\lambda_\alpha t} \tag{173}$$

provided that the operator fulfills some conditions required for the completeness of the eigenfunctions.

An interesting question arises here in connection with the asymptotic properties of these eigenvalues and eigenmodes when Ω is very large. Recently Ruijgrok and Tjon[10] gave a rigorous treatment of the eigenvalue problem of the Weiss–Ising model defined by Eqs. (15) and (16). We have also obtained the same results with a different method and have extended this to a general problem. These treatments show that the relaxation modes are, roughly speaking, classified into two types. Normally, the first type of eigenmodes have relaxation frequencies independent of ϵ and correspond to spontaneous fluctuations around an equilibrium. The second type of eigenmodes have relaxation frequencies of the order of ϵ^{-1} and describe the decay of large deviations from equilibrium. When the system is at a critical or a marginal equilibrium the first type of eigenmodes accumulate to zero frequency, which is a manifestation of the slowing-down phenomenon mentioned in the last section.

These features of relaxation modes seem to be a general property of macrosystems. In the following we discuss this rather briefly from the viewpoint developed in this work. A more detailed treatment, including a few specific examples, will be reported in a separate paper.

First we note that the classical Brownian motion is a standard but uniquely simple case. If c_1 and c_2 are given by Eq. (105) and other c_n are all zero, the stochastic operator Γ takes the form

$$\Gamma\Psi = -\frac{d}{dx}\left(\gamma x + \frac{\epsilon}{2} c_2 \frac{d}{dx}\right)\Psi \tag{174}$$

By scaling x as

$$x = \epsilon^{1/2}\xi \tag{175}$$

this is transformed into

$$\Gamma\Psi = -\frac{d}{d\xi}\left(\gamma\xi + \frac{c_2}{2}\frac{d}{d\xi}\right)\Psi \tag{176}$$

for which the eigenvalues and the eigenfunctions are

$$\lambda_l = l\gamma, \quad l = 0, 1, 2,\ldots; \qquad \Psi_l = C_l\left[\exp -\frac{x^2}{2\epsilon\sigma_e}\right] H_l\left(\frac{x}{(\epsilon\sigma_e)^{1/2}}\right) \tag{177}$$

where the H_l are Hermite polynomials.

In a classical Brownian motion everything is scaled by (175) and the relaxation frequency spectrum is constantly spaced. Any fluctuation around equilibrium and any large deviation from equilibrium can be expressed as a superposition of the eigenmodes.

This does not generally apply to an arbitrary macrosystem for which the linear law (105) does not necessarily hold. But fluctuations around a stable equilibrium are regarded as Brownian. If we scale x by (175), we find that the terms higher than the third in the Kramers–Moyal expansion can be ignored. So fluctuations of the order of $\epsilon^{1/2}$ are described by the relaxation modes (177). It should be noted that even though the linear law (114) holds for deviations of the order of ϵ^0, these deviations are not represented by the above-mentioned eigenmodes. This is a difference between a nonlinear system and a strictly linear Brownian system.

At a critical or a marginal equilibrium fluctuations are anomalous. By Eqs. (166) and (170), the Kramers–Moyal equation has the form

$$\frac{\partial P}{\partial t} = \left[\frac{\partial}{\partial x}\gamma_k x^k + \frac{\epsilon}{2}\frac{\partial^2}{\partial x^2}c_2 - \frac{\epsilon^2}{6}\frac{\partial^3}{\partial x^3}c_3 + \cdots\right] P \tag{178}$$

where $k = 3$ for a critical point and $k = 2$ for a marginal point. The proper scaling is then

$$x = \epsilon^{1/(k+1)}\xi \tag{179}$$

since the terms higher than the third on the rhs of Eq. (178) then become higher in ϵ, thus leaving

$$\Gamma\Psi = -\epsilon^{(k-1)/(k+1)}\left(\frac{\partial}{\partial \xi}\gamma_k \xi^k + \frac{c_2}{2}\frac{\partial^2}{\partial \xi^2}\right)\Psi \tag{180}$$

Putting

$$\lambda = \bar{\lambda}\epsilon^{(k-1)/(k+1)} \tag{181}$$

and

$$\Psi = \overline{\Psi}\exp\left[-\frac{\gamma_k}{(k+1)c_2}\xi^{k+1}\right] \tag{182}$$

we have then the eigenvalue equation

$$(\partial^2/\partial\xi^2)\,\overline{\Psi} + G(\bar{\lambda}, \xi)\,\overline{\Psi} = 0 \tag{183}$$

where

$$G(\bar{\lambda}, \xi) = \frac{2}{c_2}\left(\bar{\lambda} + \frac{k\gamma_k}{2}\xi^{k-1} - \frac{{\gamma_k}^2}{2c_2}\xi^{2k}\right) \tag{184}$$

We use the WKB approximation

$$\oint [G(\bar{\lambda}, \xi)]^{1/2}\, d\xi = 2\pi(l + \tfrac{1}{2}), \qquad l = 0, 1, 2,... \tag{185}$$

to determine large eigenvalues corresponding to large integers l. For a critical equilibrium the integration extends over $-\xi_1 \leqslant \xi \leqslant \xi_1$, where $\pm\xi_1$ are the roots of

$$G(\bar{\lambda}, \pm\xi_1) = 0$$

For a marginal equilibrium case x approaches zero only from the positive side, so that the integration should be limited to $0 \leqslant \xi \leqslant \xi_1$. The integration in (185) can be simplified because the second term in the brackets of Eq. (184) can be ignored in evaluating large eigenvalues. The results are asymptotic evaluations of eigenvalues as

$$\lambda_l \simeq \epsilon^{(k-1)/(k+1)} l^{2k/(k+1)} \times 2^{-1}[(2\pi)^{2k}\, \gamma_k^{\,2} c_2^{k-1} A_k^{-2k}]^{1/(k+1)} \tag{186}$$

where

$$A_3 = 4\int_0^1 (1 - \eta^6)^{1/2}\, d\eta = 2^{3/2}/3\; K(2^{-1/2}) = 1.748...$$

and

$$A_2 = 2\int_0^1 (1 - \eta^4)^{1/2}\, d\eta = 3K\frac{(\sqrt{6} - \sqrt{2})}{4} = 4.794...$$

Thus we have found that the relaxation frequencies accumulate at zero as

$$\lambda_l \propto l^{3/2}\epsilon^{1/2} \tag{187}$$

in the critical equilibrium case, and as

$$\lambda_l \propto l^{4/3}\epsilon^{1/3} \tag{188}$$

in the marginal equilibrium case. In other words, out of the normal relaxation modes (177), about $\Omega^{1/3}$ of the lower ones approach the zero frequency as the system becomes critical, and about $\Omega^{1/4}$ modes do the same as the system becomes marginal. This means that fluctuations at the critical or the marginal point are extremely long lived, which is characteristically associated with the nonlinear property at these points.

Returning to the Kramers–Moyal operator (172), we observe now that all orders of the expansion have to be retained if we come to very large quantum numbers of the order of $l \sim O(\epsilon^{-1})$, because the wavelengths of the eigenfunctions are then $O(\epsilon)$. This means that we need a more accurate analysis of Eq. (10) than by truncating Eq. (13). Here we employ the method

of large perturbations devised by Bethe[11] many years ago, which is summarized as follows.

Consider the difference eigenvalue equation

$$W(n)\,\psi(n) - A(n+\tfrac{1}{2})\,\psi(n+1) - A(n-\tfrac{1}{2})\,\psi(n-1) = \lambda\psi(n) \quad (189)$$

where the off-diagonal elements $A(n)$ and the diagonal spacings

$$\Delta(n+\tfrac{1}{2}) = W(n+1) - W(n)$$

are assumed to satisfy the conditions

$$|A(n+1) - A(n)| \ll A(n), \qquad |\Delta(n+1) - \Delta(n)| \ll \Delta(n)$$

and

$$|A(n)| < \tfrac{1}{2}W(n), \qquad n \text{ large}$$

We define

$$V(n) = [W(n) - \lambda]/2A(n) \quad (190)$$

and

$$v(n) = \cos^{-1} V(n) \quad (191)$$

and find a good approximation of the solution of (189),

$$\psi(n) = \text{const} \times [A(n)\sin v(n)]^{-1/2} \cos \int^{n} v(\nu)\,d\nu$$

in the region where

$$-1 < V(n) < 1 \quad (192)$$

Outside of this region $\psi(n)$ behaves exponentially instead of oscillating. The boundary condition is the convergence of the integral of over n. Using the WKB connection to the outer regions, the eigenvalues are determined by

$$\int_{n_1}^{n_2} v(n)\,dn = \pi(l+\tfrac{1}{2}), \qquad l = \text{integer} \quad (193)$$

where the limits n_1 and n_2 are given by

$$v(n_1) = v(n_2) = 0 \qquad \text{or} \qquad |V(n_{1,2})| = 1 \quad (194)$$

By partial integration the quantum condition (193) can be written as

$$\int_{n_1}^{n_2} \frac{nV'(n)}{[1 - V(n)^2]^{1/2}}\,dn = \pi\left(l + \frac{1}{2}\right) \quad (195)$$

Now we assume detailed balance and rewrite the transition probability (27) as

$$\begin{aligned} W(X \to X + r) &= \overline{W}(X \mid X + r) \exp \tfrac{1}{2}[\Phi_e(X + r) - \Phi_e(X)] \\ &= A(x + \tfrac{1}{2}\epsilon r) \exp[\tfrac{1}{2} r \phi_e'(x) + \tfrac{1}{4}\epsilon r^2 \phi_e''(x) + \cdots] \end{aligned} \tag{196}$$

where

$$A(x + \tfrac{1}{2}\epsilon r) = (1/\epsilon)\, \bar{w}(x)$$

and assume further, for simplicity, that a jump can only be $\pm \mid r \mid$. Then our stochastic operator is of the same form as (189), so that we can apply Bethe's method. The quantum condition now reads

$$\int_{x_1}^{x_2} \frac{xV'(x)}{[1 - V(x)^2]^{1/2}}\, dx = \pi\epsilon r \left(l + \frac{1}{2}\right) \tag{197}$$

by replacing n by $x/\epsilon r$. The integration limits are determined by

$$V(x_1) = V(x_2) = 0 \tag{198}$$

Since

$$W(X) = \sum_{\pm|r|} W(X \to X + r)$$

we have from Eq. (196)

$$\begin{aligned} V(x) = \cosh \left[\frac{r}{2}\, \phi_e'(x)\right] &- \frac{\epsilon\lambda}{2\bar{w}(x)} \\ &+ \epsilon \left\{ \frac{r^2}{4}\, \phi_e''(x) \left[\cosh \frac{r}{2}\, \phi_e'(x)\right] + \frac{r}{2} \frac{\bar{w}'(x)}{\bar{w}(x)} \sinh \left[\frac{r}{2}\, \phi_e'(x)\right] \right\} \\ &+ O(\epsilon^2) \end{aligned} \tag{199}$$

Near a stable equilibrium we have

$$\phi_e'(x) \simeq -(1/\sigma_e)(x - x_e) \qquad \text{and} \qquad \phi_e''(x) \simeq -\sigma_e^{-1} \tag{200}$$

If the eigenvalue λ is $O(\epsilon^0)$, the integration (200) is limited to

$$x - x_e = O(\epsilon^{1/2})$$

so Eq. (197) is conveniently approximated by

$$\sqrt{2} \int_{x_1}^{x_2} [1 - V(x)]^{1/2}\, dx = \pi\epsilon r(l + \tfrac{1}{2}) \tag{201}$$

in which only the quadratic term of $(x - x_e)$ is retained. Taking the first bracket on the rhs of Eq. (199), we obtain the result (177) for the eigenvalues. The second bracket only gives a shift.

The same method can be applied to a critical or a marginal equilibrium to derive the result (186).

If the eigenvalue λ is $O(\epsilon^{-1})$, on the other hand, Eq. (198) gives the integration limits x_1 and x_2 deviating from x_e in order ϵ^0. The eigenmodes with these very high quantum numbers thus extend over a finite range of x. The density of eigenvalues is given by

$$(d/d\lambda) \int_{x_1}^{x_2} \cos^{-1} V(x, \lambda)\, dx = \pi\epsilon r \rho(\lambda) \tag{202}$$

which is reduced to

$$\rho(\lambda) = \frac{1}{2\pi r} \int_{x_1}^{x_2} [1 - V^2(x, \lambda)]^{-1/2} \frac{dx}{\bar{w}(x)} \tag{203}$$

For the Weiss–Ising model the above formula gives

$$\rho(\lambda) = (1/2\pi) \int dx[(1 - x^2)^{1/2} + \cosh(\mu + \alpha x) - x \sinh(\mu + \alpha x) - \lambda]^{-1/2}$$
$$\times [(1 - x^2)^{1/2} - \cosh(\mu + \alpha x) + x \sinh(\mu + \alpha x) + \lambda]^{-1/2} \tag{204}$$

with the use of

$$\phi = \mu x + \tfrac{1}{2}\alpha x^2 - \tfrac{1}{2}(1 + x) \log[\tfrac{1}{2}(1 + x)] - \tfrac{1}{2}(1 - x) \log[\tfrac{1}{2}(1 - x)]$$

which is obtained from Eq. (17) and by assuming $\bar{w}$ to be a constant. This is identical to the result obtained by Ruijgrok and Tjon[10] using a spin operator algebra.

9. CONCLUDING REMARKS

We based our theory upon the Markovian assumption. As was mentioned in introduction, this certainly limits the direct applicability of the theory, although we conjecture that many of essential features will remain even when this restriction is removed. As a matter of principle, in many cases a Markovian model can be used, provided that a sufficient number of variables are chosen to describe the process. In practice, however, this will lead to complications. In some cases it is very essential to have a great number of variables. As long as the number is finite our description of critical phenomena cannot go beyond the mean field theory. As is well known, the delicate

singularity at a critical point comes from the interplay of an infinite set of field variables of the order parameter which results in a breakdown of the Gaussian property in long-wavenumber modes at the immediate vicinity of the critical point. Instead 822/9/1-4 verse size of the system, the wave number should appear as the parameter ϵ.

We have left a few points untouched in this paper. A useful method for dealing with a stochastic process is the so-called Langevin equation approach. A Markovian Gaussian process corresponds to a Langevin equation with Gaussian white noise. However, generally this has to be nonstationary and the noise power depends on the state of the system. This is related to the path integral representation described in this paper. Many recent treatments of nonlinear processes use the Langevin equation method. Thus our theory will be useful to obtain a deeper understaning of such approaches.

Our theory seem to have numerous applications. As mentioned earlier, many birth and death problems can be attacked with this method. Interesting applications are to nonlinear noise problems, as was studied by van Kampen some time ago. Some of these applications are in progress and will be reported on in the near future.

APPENDIX A. PATH INTEGRAL FORMULATION

The transition probability $P(x, t \mid x_0, t_0)$ from x_0 to x in a time interval $t_0 < t$ is the fundamental solution of Eq. (12) with the initial condition $P(x, t_0 \mid x_0, t_0) = \delta(x - x_0)$. This is shown to be expressed in terms of a path integral of the form

$$P(x, t \mid x_0, t_0) = \int d\mathscr{D}(x, \pi) \times \exp\left\{-\frac{1}{\epsilon}\int_{t_0}^{t} ds[H(x(s), i\pi(s), s) - i\pi(s)\,\dot{x}(s)]\right\} \tag{A.1}$$

As an asymptotic evaluation for a very small value of the parameter ϵ the above expression is transformed into another form of a path integral

$$P(x, t \mid x_0, t_0) = \int d\mathscr{D}(x) \exp\left[\frac{1}{\epsilon}\int_{t_0}^{t} ds\, L(x(s), \dot{x}(s))\right] \tag{A.2}$$

Here we defined the Hamiltonian H by

$$H(x, p, t) = \int dr\, (1 - e^{-rp})\, w(x, r, t) \tag{A.3}$$

in terms of the transition probability w, Eq. (9), and the Lagrangian L by

$$L(x, \dot{x}, t) = -H(x, p, t) + p\dot{x} \tag{A.4}$$

and

$$\partial H(x, p, t)/\partial p = \dot{x} \tag{A.5}$$

by which p is thought of as a function of x and $\dot{x}$. In (A.1) the paths are in the "phase space" of x and π and in (A.2) they are in the configuration space of x. The measure of paths in each case should be properly defined as in the case of a Feynman or a Wiener integral.

In order to see this, we first note that in the x representation

$$\begin{aligned}
&\langle x' \mid \exp[-(\Delta t/\epsilon)\, H(x', \epsilon\, \partial/\partial x', t)] \mid x'' \rangle \\
&\quad = \int_{-\infty}^{\infty} dk \exp[-(\Delta t/\epsilon)\, H(x', i\epsilon k, t) + ik(x' - x'') + O(\Delta t^2)] \qquad \text{(A.6)} \\
&\quad = \int_{-\infty}^{\infty} (d\pi/\epsilon) \exp\left\{-(\Delta t/\epsilon)\left[H(x', i\pi, t) - i\pi \frac{x' - x''}{\Delta t}\right] + O(\Delta t^2)\right\}
\end{aligned}$$

for a short time Δt, where we used the fact that the differential operator $\partial/\partial x$ appears in H only to the left of functions of x, so that the effect of non-commutability of x' and $\partial/\partial x'$ arises only in the higher order of Δt. The formal solution of Eq. (12) is now written as

$$\begin{aligned}
&P(x, t \mid x_0, t_0) \\
&\quad = \exp_{\leftarrow}\left[-\frac{1}{\epsilon}\int_{t_0}^{t} ds\, H\left(x, \epsilon \frac{\partial}{\partial x}, s\right)\right] \delta(x - x_0) \\
&\quad = \lim_{\Delta t \to 0} \exp\left[-\frac{\Delta t}{\epsilon} H\left(x, \epsilon \frac{\partial}{\partial x}, t\right)\right] \delta(x - x_{n-1})\, dx_{n-1} \\
&\qquad \times \exp\left[-\frac{\Delta t}{\epsilon} H\left(x_{n-1}, \epsilon \frac{\partial}{\partial x_{n-1}}, t_{n-1}\right)\right] \delta(x_{n-1} - x_{n-2})\, dx_{n-2} \\
&\qquad \times \cdots \\
&\qquad \times \exp\left[-\frac{\Delta t}{\epsilon} H\left(x_1, \epsilon \frac{\partial}{\partial x_1}, t_1\right)\right] \delta(x_1 - x_0)\, dx_1 \qquad \text{(A.7)}
\end{aligned}$$

where $\exp_{\leftarrow}$ means an ordered exponential, which is decomposed into a product of an infinite number of infinitesimal evolution operators of the form (A.6), and the multiplication is performed in the x representation using the expression (A.6). Thus we see that the expression

$$\begin{aligned}
P(x, t \mid x_0, t_0) = \lim_{n \to \infty} \int \cdots \int dx_1\, d\pi_1\, dx_2\, d\pi_2 \cdots dx_{n-1}\, d\pi_{n-1}\, \epsilon^{-n} \\
\times \exp\left\{-\frac{1}{\epsilon}\sum_{j=1}^{n-1} \Delta t \left[H(x_j, i\pi_j, t_j) - i\pi_j \frac{x_j - x_{j-1}}{\Delta t}\right]\right\} \\
t_j = t_0 + j\Delta t, \qquad n\,\Delta t = t - t_0, \qquad x_n = x \qquad \text{(A.8)}
\end{aligned}$$

is reduced to the path integral (A.1) in the limit $\Delta t \to 0$.

For a very small value of ϵ the path integral (A.1) can be evaluated asymptotically. Writing

$$i\pi(s) = p(s) + i\pi'(s)$$

and

$$(1/\epsilon) \int ds\, [H(x(s), i\pi(s), s) - i\pi(s)\, \dot{x}(s)]$$
$$= \sum (\Delta s_j/\epsilon)[H(x(s_j), i\pi(s_j), s_j) - i\pi(s_j)\, \dot{x}(s_j)]$$

we suppose that the time intervals Δs_j are not too small, so that the steepest descent evaluation can be used for large values of $\Delta s/\epsilon$ and that the paths are effectively limited to those sufficiently smooth for the chosen set of reasonably small intervals Δs_j to allow us to approximate the time integration by a sum over the Δs_j . Choosing the cols at

$$\partial H(x(s), p(s), s)/\partial p(s) = \dot{x}(s)$$

we perform the integrations over the $\pi'(s_j)$ to get

$$\prod_j \int d\pi'(s_j) \exp\left\{-\frac{\Delta s_j}{\epsilon}\, [H(x(s_j), i\pi(s_j), s_j) - i\pi(s_j)\, \dot{x}(s_j)]\right\}$$
$$\sim \prod_j \left(\frac{2\pi\epsilon}{-H_{pp}\, \Delta s_j}\right)^{1/2} \exp\left\{-\frac{\Delta s_j}{\epsilon}\, [H(x(s_j), p(s_j), s_j) - p(s_j)\, \dot{x}(s_j)]\right\}$$

since $H_{pp} = \partial^2 H/\partial p^2$ is negative for real values of p [see Eq. (A.3)]; this can be written as Eq. (A.2) with the Lagrangian (A.4) and with a properly defined measure of the paths in the configuration space.

By Eq. (A.3) the Hamiltonian H now is given as

$$H(x, p, t) = \sum_{n=1}^{\infty} \frac{(-)^{n-1}}{n!}\, c_n(x, t)\, p^n$$
$$= c_1(x, t)\, p - \tfrac{1}{2} c_2(x, t)\, p^2 + \cdots \tag{A.9}$$

so that Eq. (A.5) becomes

$$\dot{x} = c_1 - c_2\, p + \tfrac{1}{2} c_3\, p^2 - \cdots \tag{A.10}$$

or

$$p = p_0 + \frac{c_3}{2c_2}\, p^2 - \frac{c_4}{6c_2}\, p^3 + \cdots$$
$$= p_0 + \frac{c_3}{2c_2}\, p_0{}^2 + \left(\frac{c_3{}^2}{2c_2{}^2} - \frac{c_4}{6c_2}\right) p_0{}^3 + \cdots \tag{A.11}$$

where

$$p_0 = [c_1(x, t) - \dot{x}]/c_2(x, t) \tag{A.12}$$

Then Eq. (A.4) gives

$$L = -H + px = -c_2 \left[\frac{1}{2} p_0^2 + \frac{c_3}{6c_2} p_0^3 + \left(\frac{c_3^2}{8c_2^2} - \frac{c_4}{24c_2}\right) p_0^4 + \cdots\right] \tag{A.13}$$

The path integral (A.2) reduces to Eq. (136) if only the lowest-order term is retained in (A.13), namely

$$L(x, \dot{x}, t) = -[1/2c_2(x, t)][c_1(x, t) - \dot{x}(t)]^2 \tag{A.14}$$

APPENDIX B. THE HAMILTON–JACOBI METHOD

Another step of asymptotic evaluation can be made for the path integral (A.2) by choosing the path that maximizes the action integral

$$J(t, t_0) = J(x, t \mid x_0, t_0) = \int ds\, L(x, \dot{x}, s) \tag{B.1}$$

The path is determined by the Euler equation,

$$\frac{d}{ds}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0 \tag{B.2}$$

or by the canonical equations of motion

$$\dot{p}(s) = -\partial H/\partial x, \qquad \dot{x}(s) = \partial H/\partial p \tag{B.3}$$

with the conditions

$$x(t_0) = x_0 \qquad \text{and} \quad x(t) = x \tag{B.4}$$

In the phase space (x, p) such a path may or may not be found by a suitable choice of the initial value $p_0 = p(t_0)$. If it can be found, the action integral (B.1) gives the required transition probability by

$$P(x, t \mid x_0, t_0) = C \exp[(1/\epsilon)\, J(x, t \mid x_0, t_0)] \tag{B.5}$$

as an asymptotic expression for a small value of ϵ. This is another way of looking at the asymptotic nature of our problem and is in accordance with what we have discussed in the text.

One immediately notes now that this is closely related to Eq. (78). If we write

$$\partial\phi_0/\partial x = p \qquad \text{and} \qquad \partial\phi_0/\partial t = q$$

Eq. (78) is simply written as

$$q + H(x, p, t) = 0 \tag{B.7}$$

The characteristic equations of this partial differential equation are

$$\begin{aligned} &\frac{dx}{dt} = \frac{\partial H}{\partial p}, \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial x} \\ &\frac{dJ}{dt} = q + p\frac{\partial H}{\partial p} = -H + p\frac{\partial H}{\partial p} \equiv L, \qquad \frac{dq}{dt} = -\frac{\partial H}{\partial t} \end{aligned} \tag{B.8}$$

where we write J for ϕ_0 in Eq. (78). The first two equations are of course identical with (B.3) and the third with (B.1).

The Cauchy problem of Eq. (78) is solved by the standard method in the following way. At $t = t_0$ we impose the initial conditions

$$\begin{aligned} &x(t_0) = \xi, \qquad p(t_0) = f'(\xi), \qquad J(t_0) = f(\xi) \\ &q(t_0) = -H(\xi, f'(\xi), t_0) \end{aligned} \tag{B.9}$$

and find the solutions of the ordinary differential equations (B.8) as

$$x = x(t, \xi), \qquad p = p(t, \xi), \qquad J = J(t, \xi), \qquad q = q(t, \xi) \tag{B.10}$$

These solutions give $J(x, t)$ as the solution of Eq. (78) in a parametric representation through ξ. At $t = t_0$ we have imposed the initial function

$$J(x, t_0) = f(x) \tag{B.11}$$

and at time t we find $J(x, t)$ by

$$x = x(t, \xi) \qquad \text{and} \qquad J = J(t, \xi) \tag{B.12}$$

If the basic process is stationary in the sense that H does not depend on t explicitly, the conservation law then holds

$$H(x, p) = \text{const} = H(\xi, f'(\xi)) \tag{B.13}$$

which can be solved in p to express it in terms of x and ξ. Then the first equation of (B.8) is integrated to give

$$\int_{\xi}^{x} \frac{dx}{\partial H/\partial p} = t - t_0 \tag{B.14}$$

and the third to give

$$J(t) = f(\xi) - H(\xi, f'(\xi))\, t + \int_{\xi}^{x} p\, dx \tag{B.15}$$

These two equations yield $J(x, t)$ at time t.

This can be conveniently visualized in the phase space (x, p). The Hamiltonian $H(x, p)$ induces flows in the phase space. The function $J(x, t)$ is there represented by a front which expresses the relationship between x and p as determined by the first two equations in (B.10). The initial front is thus the curve $p = f'(x)$ and it propagates in time according to the phase flow. If there exists an equilibrium distribution $P_{eq}(x)$, the front approaches the corresponding final front.

This is most easily illustrated by the simple example of a Brownian motion, for which we have

$$c_1(x) = -\gamma x \qquad \text{and} \qquad c_2 = \text{const} = c$$

so that the Hamiltonian H is

$$H = -\gamma x p - \tfrac{1}{2} c p^2 \tag{B.16}$$

The constant-H contours in the phase space are shown in Fig. 2. The straight lines

$$p = 0 \qquad \text{and} \qquad p + (2\gamma/c)\, x = 0$$

are those for $H = 0$. Between these straight lines there are flows with $H > 0$ or $H > 0$ as indicated in the figure. The arrows show the directions of the flow. If the initial function is

$$J(x, t) = -(1/2\sigma_0)(x - x_0)^2$$

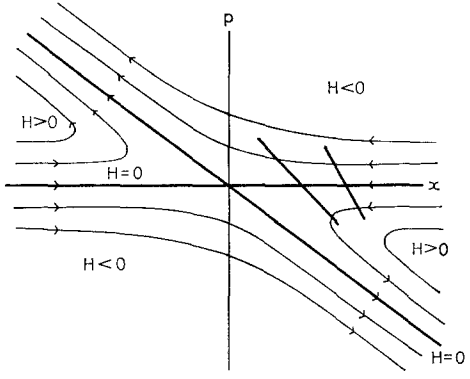

Fig. 2. Phase flow for a Brownian system.

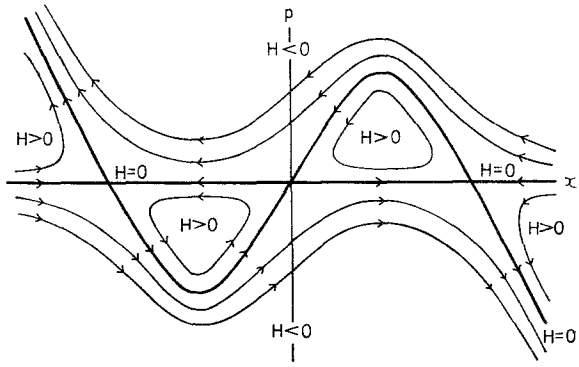

Fig. 3. Phase flow for a ferromagnet below the critical point.

corresponding to an initial Gaussian distribution of P, the initial front is

$$p = -(1/\sigma_0)(x - x_0)$$

In this simple case Eq. (B.8) are very easily solved. The front remains a straight line

$$p = -(1/\sigma_t)(x - x_0 e^{-\gamma t}), \qquad \sigma_t = \sigma_e + (\sigma_0 - \sigma_e)\, e^{-2\gamma t}$$

at later times and approaches the final asymptote

$$p = -(2\gamma/c)\, x = -(1/\sigma_e)\, x$$

at $t = \infty$, corresponding to the equilibrium distribution (108).

In a general case there may be stable and unstable equilibrium points of x and the flow pattern in the phase space may be more complex. An example is illustrated in Fig. 3, which corresponds to a ferromagnet below the Curie temperature. By Eq. (A.9) the straight line $p = 0$ is the contour with $H = 0$. There is another contour with $H = 0$ as shown in the figure, which defines domains of phase flow. The temporal evolution of $\phi_0(x, t)$ in Eq. (78) is determined by this sort of flow pattern. This will be discussed in more detail in a forthcoming paper.

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