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On the Construction of a Time-Reversed Markoff Process

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For a given Markoff process characterized by a set of transition probability densities there exists another process with time reversed (the ***retrodictive*** vs ***predictive*** process in the theory of measurements) such that any one of them multiplied by a single-event density may be symmetric with respect to an interchange of the events expressed as space-time variables, yielding a joint probability density. It is shown how this time-reversed process can be constructed by means of the generating operator of the associated evolution equation, and the basic properties with explicit applications to master equations and Fokker-Planck equations. Onsager's microscopic reversibility is reformulated on this basis. Possible symmetries concerning time-correlation functions under the Markoffian law is summarized in comparion with the Kubo formula. In the application to Fokker-Planck equations, the Onsager-Machlup most probable paths are extended to general type of diffusion processes, and it is shown that the present method corresponds to a gauge transformation in dynamics of a charged particle which leaves its paths invariant.

§ 1. Introduction

Reciprocity has been a fundamental subject in the theory of irreversible processes, since Onsager initiated the approach to the problem based on the consideration of *microscopic reversibility*.[1] The Onsager relations for a linear dissipative system in an external magnetic field Θ, given by $L_{\mu\nu}(-\Theta)=L_{\nu\mu}(\Theta)$, have since been discussed in a number of papers. Kubo's general linear response theory[2] among them provided an accurate statistical-mechanical foundation of these relations, expressing the microscopic reversibility in the time correlation functions between Hamiltonian-driven dynamical variables.

Recently, the interests have been revised in connection with the statistical mechanics for non-equilibrium or open systems far from equilibrium conditions. Van Kampen discussed a possibility of extending the relations straightforwardly to the nonlinear regime of flux-force equations.[3] Another systematic approach has been developed by using equations of evolutions for probability densities based on the theory of Markoff processes.[4] An interesting finding in the latter approach has been that the microscopic reversibility as represented by a form of *detailed balance* condition (or its equivalent) is a situation rather restrictive for such non-equilibrium states: There exist a number of important examples of violation such as complex optical systems and chemical reactions. A typical non-trivial system, a single-mode laser, is a special example for which the *potential condition* equivalent to the reversibility is well satisfied, as discussed by Graham and Haken.[5]

This led Tomita and his associates to investigate actively the so-called "irreversible circulation" phenomena.[6)~8)] On the other hand, Hepp has very recently pointed out that the detailed balance should be originated, when an open system is formulated as a small dynamical system coupled weakly with several large reservoirs, from the Kubo-Martin-Schwinger (KMS) condition for the reservoirs irrespective of the usual time-reversal operation and hence that the Onsager relations result without recourse to the microscopic reversibility.[9)]

In this paper, we propose a formal scheme to construct a time-reversed set of evolution equations in place of the microscopic reversibility in the theory of Markoff processes. The idea is originated from Nelson.[10)] This is to give an answer to the question how to connect an elementary solution of e.g., a Fokker-Planck equation "smoothly" to the one in the opposite time direction. A more explicit illustration of the problem is given in § 2. Needs for such a scheme are, firstly, to contribute to a new method of stochastic approach to non-equilibrium states by means of *trajectories* and, secondly, to establish Onsager's principle for a joint probability density from quite a general standpoint.*) In § 3 we present the method, where a notable dual structure between a process and its time-reversed one is demonstrated. Applications are made in § 4 to a master equation and a Fokker-Planck equation. For the latter example the scheme is shown to have a close analogy to a gauge transformation in the classical dynamics for a charged particle in electromagnetic fields, such that the proposed scheme assures the invariance of the equations of motion for the Onsager-Machlup deterministic trajectories[12)] (the so-called "most probable paths"). It will be usefull for studies of irreversible circulations, where Graham and Haken's potential condition[5)] is explicitly violated. The microscopic reversibility is thus reformulated from the present standpoint in § 5. Hepp's remark is incorporated into the scheme. In the final section all the possible symmetry relations regarding the Markoffian correlation functions are summarized.

§ 2. Simple illustration

Let us consider a Gaussian-Markoff process in one-dimension corresponding to a simple exponential damping (Smoluchowski process):

$$\frac{dx}{dt} = -\gamma x\,, \qquad \gamma > 0\,. \tag{2·1}$$

A probability density with which the underlying Brownian motion is averaged to yield above damping law is given by[13)]

$$P(x|x_0;\, t) = \frac{1}{\sqrt{(2\pi D/\gamma)(1-e^{-2\gamma t})}} \exp\left\{-\frac{\gamma}{2D}\frac{(x-x_0 e^{-\gamma t})^2}{1-e^{-2\gamma t}}\right\} \tag{2·2}$$

*) A part of this work has been submitted by the present author to Prog. Theor. Phys.[11)] A comprehensive treatment is in preparation.

for

$$t>0\,. \tag{2·2a}$$

In fact, the dynamical variable x is averaged over the ensemble such that

$$\langle x\rangle=\int_{-\infty}^{\infty}xP(x|x_0;\,t)\,dx\,, \tag{2·3}$$

which obeys the same equation of motion as (2·1). More generally, one can write for any physical quantity $f(x)$

$$\langle f(x)\rangle=\int_{-\infty}^{\infty}f(x)\,P(x|x_0;\,t)\,dx\,. \tag{2·4}$$

As is well-known, the function P in (2·2) represents an elementary solution of a Fokker-Planck equation

$$\frac{\partial\psi}{\partial t}=\frac{\partial}{\partial x}(\gamma x\psi)+D\frac{\partial^2\psi}{\partial x^2}\,,\qquad D>0 \tag{2·5}$$

with the initial condition

$$\psi(x,t=0)=\delta(x-x_0)\,. \tag{2·6}$$

Denoting the linear operator on ψ on the right-hand side of Eq. (2·5) by A^+ (regarded as the adjoint of A defined in Eq. (2·8)), we can write

$$\begin{aligned}\frac{d}{dt}\langle f(x)\rangle&=\int_{-\infty}^{\infty}f(x)\frac{\partial}{\partial t}P(x|x_0;\,t)\,dx=\int_{-\infty}^{\infty}f(x)\,(A^+P)\,(x)\,dx\\&=\int_{-\infty}^{\infty}((Af)P)\,(x)\,dx=\langle (Af)\,(x)\rangle\,,\end{aligned} \tag{2·7}$$

which enables us to express the evolution equation in the form

$$\frac{\partial f}{\partial t}=-\gamma x\frac{\partial f}{\partial x}+D\frac{\partial^2 f}{\partial x^2}\equiv Af\,. \tag{2·8}$$

Clearly, the Fokker-Planck equation (2·5) by itself tells nothing about its solution in the negative side of time $t<0$ which may or may not continue to the form (2·2). On the other hand, the damping behaviour given by Eq. (2·1) is considered as a consequence of continual fluctuations in the underlying open system, and sometimes it is desirable to inquire into such fluctuations in the past.

What one expects physically is that the dynamical variable x should be damped in the opposite time-direction as well after a lapse of long time *from present to past.* On this physical ground, one may look at the evolution equation for the dynamical quantity $f(x)\,(t<0)$ by reversing the sign of the derivative operation, thus

$$-\frac{\partial f}{\partial t}=Af\,. \tag{2·9}$$

This equation, called Kolmogoroff's backward equation, is necessarily related to the forward equation (2·5):

$$\frac{\partial \psi}{\partial t} = A^{+}\psi\,, \quad t>0\,, \tag{2·10}$$

because its elementary solution with the initial condition (2·6) can be expressed in terms of P in (2·2), so that[4),5)]

$$f(xt, x_0) = P(x_0|x; -t), \quad t<0\,. \tag{2·11}$$

However, there is in general no guarantee of connecting the elementary solution of the time-reversed F-P equation

$$-\frac{\partial \psi_*}{\partial t} = A^{+}\psi_*\,, \quad t<0 \tag{2·12}$$

with the above P.

It is a detailed balance condition that makes it possible to relate the two solutions of Eqs. (2·10) and (2·12) via the backward solution (2·11). To see this, let us recall the special relation satisfied between the two linear differential operators A and A^+, namely (a kind of canonical transformation by an operator ρ_0[10)])

$$A = \rho_0^{-1} A^{+} \rho_0\,, \tag{2·13}$$

where ρ_0 is the steady-state solution of Eq. (2·5):

$$A^{+}\rho_0 = 0\,. \tag{2·13a}$$

We can then set, for a solution of Eq. (2·12),

$$\psi_*(xt) = f(xt)\rho_0(x) \tag{2·14}$$

by virtue of Eqs. (2·9), (2·13) and (2·13a). In particular, the elementary solution of Eq. (2·12) with the initial condition

$$\psi_*(x, t=0) = \delta(x-x_0) \tag{2·15}$$

can be expressed by means of the expression (2·11) as

$$P_*(x|x_0; t) = P(x_0|x; -t) \times \frac{\rho_0(x)}{\rho_0(x_0)}\,. \tag{2·16}$$

This last equation shows a sort of detailed balance, but not in the sense of Graham and Haken,[5)] since it does not involve the time-reversal operation on the dynamical variables.

The existence of the relation (2·13), a special privilege for the simplicity of the present example (equivalent to saying that the operator A is symmetrizable), cannot be expected generally. However, we may consider the relation (2·16) as more fundamental than (2·13): in other words, there exists a general ground that Eq. (2·16) holds without recourse to the symmetrizability (2·13). In the following we will show this assertion.

§ 3. General scheme

We formulate the problem, starting with two sets of equation of evolution each consisting of the one for a probability density and its adjoint with the time-derivative operation reversed, as motivated by the foregoing argument. The first set of equation reads:

$$\frac{\partial \psi}{\partial t} = A^{+}\psi\,, \tag{3·1}$$

$$-\frac{\partial f}{\partial t} = Af\,. \tag{3·1'}$$

For the second set, we write

$$-\frac{\partial \psi_*}{\partial t} = A_*{}^{+}\psi_*\,, \tag{3·2}$$

$$\frac{\partial f_*}{\partial t} = A_* f_*\,. \tag{3·2'}$$

The two linear operators A_* and $A_*{}^{+}$ must in some way be related to A and A^{+}, as an extension of Eq. (2·13), which we now seek.

These operators should satisfy the conditions:

i) A^{+} and A are both dissipative operators.

ii) $A1=0$ (vanishing, when operated on unity).

The condition i) demands that the operators A^{+} and A are of negative character,*) so that

$$[A^{+}\psi,\,\psi]\leq 0 \quad \text{and} \quad [Af, f]\leq 0 \tag{3·3}$$

for any semi-scalar product[14] (expressed as a square bracket) definable in the respective ψ- and f-spaces just as the usual scalar product in a Hilbert space. The condition ii) is the physical requirement that the total probability (integral of ψ) is time-independent, normalizable to unity.

We now show that the following procedure will give an answer for finding $A_*{}^{+}$ and A_*. We multiply ψ by a certain element, which we designate as $e^{-\theta}$, and try to produce an evolution equation for $e^{-\theta}\psi$ with the aid of Eqs. (3·1), (3·1'):

$$\frac{\partial}{\partial t}(e^{-\theta}\psi) = e^{-\theta}\frac{\partial \psi}{\partial t} + \left(\frac{\partial}{\partial t}(e^{-\theta})\,\psi\right) = \left(e^{-\theta}A^{+}e^{\theta} - \frac{\partial \theta}{\partial t}I\right)e^{-\theta}\psi\,,$$

where I denotes the identity operator. We assume that $e^{-\theta}$ is a continuous, dif-

*) See Note added in proof 1.

ferentiable function for t and, furthermore, $e^{-\theta}\psi$ is a linear operation on the space of ψ. Hence, the operator

$$A_\theta \equiv e^{-\theta}A^+e^\theta - \frac{\partial\theta}{\partial t}I \tag{3·4}$$

generates a time evolution of $e^{-\theta}\psi$ in the $+$ direction. Let it satisfy the two conditions, i) and ii). The latter condition reads

$$A_\theta 1 = e^{-\theta}A^+(e^\theta) - \frac{\partial\theta}{\partial t} = 0 \qquad \therefore \quad e^\theta\frac{\partial\theta}{\theta t}\left(=\frac{\partial}{\partial t}e^\theta\right) = A^+(e^\theta).$$

Denoting e^θ by ρ_0, we have

$$\frac{\partial\rho_0}{\partial t} = A^+\rho_0\,. \tag{3·5}$$

Thus, there exists a positive solution ρ_0 of Eq. (3·1) which enables us to write with a real θ as

$$\rho_0 = e^\theta \quad (\text{or } \theta = \log\rho_0). \tag{3·6}$$

Also, with this e^θ, we have for the second evolution equation

$$-\frac{\partial}{\partial t}(e^\theta f) = -e^\theta\left(\frac{\partial f}{\partial t} + \frac{\partial\theta}{\partial t}f\right) = \left(e^\theta Ae^{-\theta} - \frac{\partial\theta}{\theta t}I\right)e^\theta f\,,$$

which generates a time evolution in the $-$ direction, the generator being identified with $A_\theta{}^+$ by virtue of Eq. (3·4), i.e.,

$$A_\theta{}^+ = e^\theta Ae^{-\theta} - \frac{\partial\theta}{\partial t}I\,. \tag{3·4'}$$

In order to see condition i), i.e., the dissipative property of the transformed operators A_θ and $A_\theta{}^+$, let us consider a semi-scalar product $[A_\theta{}^+\psi_*, \psi_*]$ and also $[A_\theta f_*, f_*]$ in the transformed spaces of $\psi_* = e^\theta f$ and $f_* = e^{-\theta}\psi$, respectively:

$$[A_\theta{}^+\psi_*, \psi_*] = [Af, e^{2\theta}f] - \left[\frac{\partial\theta}{\partial t}f, e^{2\theta}f\right],$$

$$[A_\theta f_*, f_*] = [A^+\psi, e^{-2\theta}\psi] - \left[\frac{\partial\theta}{\partial t}\psi, e^{-2\theta}\psi\right].$$

Since $e^{2\theta}(e^{-2\theta})$ is a positive quantity, an expression $[g, e^{2\theta}f]$ ($[\varphi, e^{-2\theta}\psi]$) can be regarded as another semi-scalar product in the f-(ψ-) space. Therefore, the dissipative conditions for $A_\theta{}^+$ and A_θ reduce to

$$[Af, f] \leq \left[\left(\frac{\partial}{\partial t}\log\rho_0\right)f, f\right] \quad \text{and} \quad [A^+\psi, \psi] \leq \left[\left(\frac{\partial}{\partial t}\log\rho_0\right)\psi, \psi\right] \tag{3·7}$$

with *any* semi-scalar product in the f- and ψ-spaces, respectively. In particular, if ρ_0 is the steady-state solution for which $\partial\rho_0/\partial t=0$, the inequalities in (3·7) are assured by the dissipative conditions for A and A^+, (3·3).

The above result is now summarized:

(1) *The time-reversed evolution equations* (3·2), (3·2′) *with property* ii) *can be established by setting*

$$A_*^+=\rho_0 A\rho_0^{-1}-\frac{(A^+\rho_0)}{\rho_0}I\,, \tag{3·8}$$

$$A_*=\rho_0^{-1}A^+\rho_0-\frac{(A^+\rho_0)}{\rho_0}I\,, \tag{3·8′}$$

where ρ_0 *is an arbitrary solution of* $\partial\rho_0/\partial t=A^+\rho_0$. *If further,* ρ_0 *is the steady-state solution* $A^+\rho_0=0$, *the generating operators* A_*^+ *and* A_* *may also have property* i). *Their solutions may be obtained from the original evolution equations* (3·1), (3·2) *by*

$$\psi_*=\rho_0 f\,,\qquad f_*=\frac{\psi}{\rho_0}\,. \tag{3·9}$$

We next show that our scheme has a dual structure. That is, schematically

$$(A^+,A)\xrightarrow{\rho_0}(A_*^+,A_*)\xrightarrow{\rho_0}((A_*^+)_*=A^+,\ (A_*)_*=A)\,.$$

Thus, we have the following:

(2) *The process of time-reversing* $(A^+,A)\xrightarrow{\rho_0}(A_*^+,A_*)$ *has a reflexive property*

$$(A_*^+)_*=A^+\,,\qquad (A_*)_*=A\,, \tag{3·10}$$

where the ρ_0 *satisfies not only*

$$\frac{\partial\rho_0}{\partial t}=A^+\rho_0 \tag{3·11}$$

but also the time-reversed equation

$$-\frac{\partial\rho_0}{\partial t}=A_*^+\rho_0\,. \tag{3·11′}$$

For the proof we operate with A_*^+ given by (3·8) on ρ_0 to obtain

$$A_*^+\rho_0=\rho_0(A1)-A^+\rho_0=0-A^+\rho_0=-\frac{\partial\rho_0}{\partial t}\,,$$

by virtue of property ii) and Eq. (3·11). Thus, we substitute A_* and A_*^+ for A and A^+, respectively, on the right-hand sides of Eqs. (3·8), (3·8′) to get $(A_*)_*$ and $(A_*^+)_*$, in such a way that

$$(A_*)_*=\rho_0^{-1}A_*^+\rho_0-\frac{(A_*^+\rho_0)}{\rho_0}I$$

$$=\rho_0^{-1}\left(\rho_0 A\rho_0^{-1}-\frac{(A^+\rho_0)}{\rho_0}I\right)\rho_0-\frac{\rho_0(A1)-(A^+\rho_0)}{\rho_0}I$$

$$=A-\frac{(A^+\rho_0)}{\rho_0}I+\frac{(A^+\rho_0)}{\rho_0}I=A$$

and similarly

$$(A_*^{+})_*=A^+ ,$$

which proves the relations in (3·10). Also, the two relations given in (3·9) themselves complement the reflexivity of solutions: $\psi=\rho_0 f_*=(\psi_*)_*$, and $f=\psi_*/\rho_0=(f_*)_*$. This completes the proof.

§ 4. Application to a master equation and a Fokker-Planck equation

4A. *Master equation*

$$\frac{\partial}{\partial t}\psi(xt)=\int A^+(xx')\psi(x't)dx'$$

$$=\int(W(xx')\psi(x't)-W(x'x)\psi(xt))dx' , \qquad (4\cdot1)$$

$$-\frac{\partial}{\partial t}f(xt)=\int f(x't)A(x'x)dx'$$

$$=\int(f(x't)-f(xt))W(x'x)dx' . \qquad (4\cdot1')$$

The kernel representation of the operator A is expressed by a transition probability rate $W(>0)$ as

$$A(x'x)=A^+(xx')=W(xx')-\delta(x-x')\int W(x''x)dx'' . \qquad (4\cdot2)$$

Formula (3·8′) is now used to obtain the expression for $A_*(xx')$ as follows:

$$A_*(xx')=\frac{1}{\rho_0(x)}\left(A^+(xx')\rho_0(x')-\int\rho_0(x'')A(x''x)dx''\delta(x-x')\right)$$

$$=W(xx')\frac{\rho_0(x')}{\rho_0(x)}-\delta(x-x')\int W(x''x)\frac{\rho_0(x'')}{\rho_0(x)}dx''. \qquad (4\cdot3)$$

This shows that the time-reversed master equation associated with Eqs. (4·1), (4·1′) may be represented as

$$-\frac{\partial}{\partial t}\psi_*(xt)=\int(W_*(xx')\psi_*(x't)-W_*(x'x)\psi_*(xt))dx' , \qquad (4\cdot4)$$

$$\frac{\partial}{\partial t}f_*(xt)=\int(f_*(x't)-f_*(xt))W_*(x'x)dx' , \qquad (4\cdot4')$$

where the transition probability rate is given by

$$W_*(x'x) = W(xx') \times \frac{\rho_0(x')}{\rho_0(x)}\,. \tag{4·5}$$

The result implies that the transition probability rate W is to be transformed by ρ_0 just as the transition probability density P, where $\rho_0(xt)$ is one solution of Eq. (4·1) in accordance with the general prediction. In the above, the t-dependence of ρ_0 is not explicitly indicated. If it is actually t-independent, it must be a steady-state, i.e.,

$$\int (W(xx')\rho_0(x') - W(x'x)\rho_0(x))\,dx' = 0\,. \tag{4·6}$$

4B. *Fokker-Planck equation*

$$\frac{\partial}{\partial t}\psi(xt) = -\frac{\partial}{\partial x_\mu}(v_\mu \psi) + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial}{\partial x_\nu}\psi\right), \tag{4·7}$$

$$-\frac{\partial}{\partial t}f(xt) = v_\mu \frac{\partial}{\partial x_\mu}f + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial}{\partial x_\nu}f\right), \tag{4·7$'$}$$

where the summation convention of dummy suffix has been used. In Eqs. (4·7), (4·7′), the vector v_μ and the tensor $D_{\mu\nu}$ are the drift velocity and the diffusion coefficients, respectively, and may be in general space-time functions. The diffusion tensor $D_{\mu\nu}$ is of a symmetric, non-negative type ($D_{\mu\nu}u_\mu u_\nu \geq 0$ for any real vector u_μ). There must exist some condition imposed also on the drift velocity v_μ for stable solutions, which we will not go into here.

The transformations defined in Eqs. (3·8), (3·8′) are performed on the differential operators for the Fokker-Planck eqations (4·7), (4·7′), i.e.,

$$A^+ = -\frac{\partial}{\partial x_\mu}v_\mu + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial}{\partial x_\nu}\right), \qquad A = v_\mu \frac{\partial}{\partial x_\mu} + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial}{\partial x_\nu}\right)$$

in the following manner:

$$\begin{aligned} e^{-\theta}A^+e^\theta &= A^+ - v_\mu \frac{\partial\theta}{\partial x_\mu} + 2D_{\mu\nu}\frac{\partial\theta}{\partial x_\mu}\frac{\partial}{\partial x_\nu} + D_{\mu\nu}\frac{\partial\theta}{\partial x_\mu}\frac{\partial}{\partial x_\nu} + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial\theta}{\partial x_\nu}\right) \\ &= \left(-v_\mu + 2D_{\mu\nu}\frac{\partial\theta}{\partial x_\nu}\right)\frac{\partial}{\partial x_\mu} + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial}{\partial x_\nu}\right) \\ &\quad -\frac{\partial v_\mu}{\partial x_\mu} - v_\mu\frac{\partial\theta}{\partial x_\mu} + D_{\mu\nu}\frac{\partial\theta}{\partial x_\mu}\frac{\partial\theta}{\partial x_\nu} + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial\theta}{\partial x_\nu}\right) \end{aligned}$$

and

$$\frac{(A^+e^\theta)}{e^\theta} = \frac{\partial\theta}{\partial t} = -\frac{\partial v_\mu}{\partial x_\mu} - v_\mu\frac{\partial\theta}{\partial x_\mu} + D_{\mu\nu}\frac{\partial\theta}{\partial x_\mu}\frac{\partial\theta}{\partial x_\nu} + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial\theta}{\partial x_\nu}\right). \tag{4·8}$$

Thus, by setting $e^\theta = \rho_0$, we have

$$A_* = \rho_0{}^{-1} A^+ \rho_0 - \frac{(A^+\rho_0)}{\rho_0} = v_{*\mu}\frac{\partial}{\partial x_\mu} + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial}{\partial x_\nu}\right), \tag{4·9}$$

where

$$v_{*\mu} = -v_\mu + 2D_{\mu\nu}\frac{\partial}{\partial x_\nu}\log\rho_0\,, \tag{4·9a}$$

and therefore

$$-\frac{\partial}{\partial t}\psi_*(xt) = -\frac{\partial}{\partial x_\mu}(v_{*\mu}\psi_*) + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial}{\partial x_\nu}\psi_*\right), \tag{4·10}$$

$$\frac{\partial}{\partial t}f_*(xt) = v_{*\mu}\frac{\partial}{\partial x_\mu}f_* + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial}{\partial x_\nu}f_*\right). \tag{4·10'}$$

This shows that the time-reversed transformation affects only the drift velocity v_μ in the first-order part to change in such second order differential operators, as given by Eq. (4·9a).

We now show that the above transformation makes the "most probable path" of Onsager and Machlup[12] invariant. The Onsager-Machlup Lagrangian with which the Fokker-Planck equation (4·7) is associated can be deduced either by a method of path integrals or by the following consideration: That is, when it is assumed to have the form

$$L(\dot{x}, xt) = \frac{1}{4}D^{-1}_{\mu\nu}\dot{x}_\mu\dot{x}_\nu - \frac{1}{2}D^{-1}_{\mu\nu}\dot{x}_\mu v_\nu - U(xt), \tag{4·11}$$

the "scalar potential" U can be fixed so that the resulting backward equation may have a trivial solution $f=1$, as shown in (4·7′). The result yields explicitly

$$U(xt) = -\frac{1}{4}D^{-1}_{\mu\nu}v_\mu v_\nu - \frac{1}{2}\frac{\partial v_\mu}{\partial x_\mu}, \tag{4·12}$$

and hence[11),*)]

$$L(\dot{x}, xt) = \frac{1}{4}D^{-1}_{\mu\nu}(\dot{x}_\mu - v_\mu)(\dot{x}_\nu - v_\nu) + \frac{1}{2}\frac{\partial v_\mu}{\partial x_\mu}, \tag{4·11'}$$

where D^{-1} stands for the inverse of D so that $D^{-1}_{\mu\nu}D_{\nu\lambda} = \delta_{\mu\lambda}$. This Lagrangian exhibits a property of covariance, when the velocity components change analogously to the gauge transformation in electrodynamics, such that the substitution

$$v_\mu \to \bar{v}_\mu = v_\mu - 2D_{\mu\nu}\frac{\partial\theta}{\partial x_\nu}, \qquad U \to \bar{U} = U - \frac{\partial\theta}{\partial t} \tag{4·13}$$

induces

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*) This result conforms to the OM Lagrangian obtained by Graham[4] apart from two additional terms in the latter, which is originated from the transformation from Cartesian to a curvilineal coordinates in the latter treatment. See also Note added in proof 2.

$$L \to \bar{L} = L + \left(\dot{x}_\mu \frac{\partial \theta}{\partial x_\mu} + \frac{\partial \theta}{\partial t}\right) = L + \frac{d\theta}{dt}\,. \tag{4·13'}$$

By virtue of the special relation between U and v_μ (the "scalar" and "vector" potentials, respectively) expressed as (4·12), however, the transformation demands that the gauge function θ must satisfy a certain partial differential equation: Only the satisfaction of such an equation may admit the transformed Lagrangian $\bar{L}$ to be of the form in (4·13') and hence $\bar{L}-L$ to be equal to $d\theta/dt$, which makes the resulting equation of motion for trajectories invariant.

There are in general two classes of such transformation: the one preserving, and the other reversing, the direction of time. In the first class the transformed Lagrangian is given by

$$\bar{L}(\dot{x}, xt) = \frac{1}{4} D_{\mu\nu}^{-1} (\dot{x}_\mu - \bar{v}_\mu)(\dot{x}_\nu - \bar{v}_\nu) + \frac{1}{2} \frac{\partial \bar{v}_\mu}{\partial x_\mu} \tag{4·14}$$

with $\bar{v}_\mu$ given in (4·13), whereas in the second by

$$\bar{L}(\dot{x}, xt) = \frac{1}{4} D_{\mu\nu}^{-1} (\dot{x}_\mu + v_{*\mu})(\dot{x}_\nu + v_{*\nu}) + \frac{1}{2} \frac{\partial v_{*\mu}}{\partial x_\mu} \tag{4·14'}$$

with $v_{*\mu}$ defined by reversing the sign of $\bar{v}_\mu$, i.e.,

$$v_{*\mu} = -\bar{v}_\mu = -v_\mu + 2D_{\mu\nu} \frac{\partial \theta}{\partial x_\nu}\,. \tag{4·15}$$

In the latter case, one is ready to observe that the required condition for θ is identified with the partial differential equation (4·8) and that the velocity $v_{*\mu}$ in (4·15) with the one given in (4·9a) by the use of the relation $\theta = \log \rho_0$.

Therefore, we can say that every Fokker-Planck equation can be characterized by a Newtonian equation of motion for its associated Onsager-Machlup trajectories, and any two different F-P equations belonging to the same Newtonian can be transferred to each other through a gauge transformation of the above-illustrated nature. The transformation corresponds physically to a change of the frame of description, such as from a static frame to a moving frame discussed by Tomita et al.[7]

§ 5. The microscopic reversibility

Let us classify broadly-used terminology "detailed balance condition" into two specified kinds: with and without time-reversal operation on the dynamical variables. Let the latter be designated as the first kind and the former as the second kind.

Detailed balance of the 1st kind. This situation occurs when the following condition is met.

$$A_* = A\,. \tag{5·1}$$

That is to say, the time-reversed generating operator is just equal to the original one for a given Markoff process. This condition when combined with the fact that the auxiliary element ρ_0 must satisfy both evolution equations (3·11), (3·11′) requires that (a) the ρ_0 must be a steady-state solution

$$A^+\rho_0(=A_*^+\rho_0)=0\,, \tag{5·2}$$

and hence

(b)
$$A=\rho_0^{-1}A^+\rho_0 \tag{5·3}$$

or, the generating operator is symmetrizable, that is,

$$\rho_0^{1/2}A\rho_0^{-1/2}=(\rho_0^{1/2}A^+\rho_0^{-1/2})^+\,. \tag{5·3′}$$

These relations result in the well-known form

$$P(x|x_0;\ t)\rho_0(x_0)=P(x_0|x;\ t)\rho_0(x) \tag{5·4}$$

for the transition probability density $P(x|x_0;\ t)$, i.e., the elementary solution of the evolution equation for ψ with the δ-type initial condition at $t=0$.

Detailed balance of the 2nd kind. The situation can be expressed as

$$A_*=\tilde{A}\,, \tag{5·5}$$

where the operator on the right-hand side, $\tilde{A}$, is defined by the time reversal of A to be performed on its dynamical variables.

Following the notation used by Graham and Haken,[5] we express the operation for each variable as

$$x_\mu\to\tilde{x}_\mu=\varepsilon_\mu x_\mu\,,^{*)} \tag{5·6}$$

where

$$\varepsilon_\mu=+1 \quad \text{or} \quad -1\,, \tag{5·6a}$$

according to Case x_μ be even and Case x_μ be odd, respectively, with respect to the operation. Further, any scalar, vector and tensor function of the variables, and consequently, an operator A represented in terms of them may have its time-reversal conjugate such that

$$f\to\tilde{f}:\quad \tilde{f}(x)=f(\tilde{x}) \tag{5·7}$$

for a scalar function $f(x)$, etc.

Now, Onsager's microscopic reversibility corresponds to the detailed balance of the latter kind, and may be expressed formally as follows:

$$\rho_{0t}\tilde{P}_t=P_t^+\rho_{0t=0}\,. \tag{5·8}$$

In this expression $\tilde{P}_t$ represents the time reversal conjugate and P_t^+ the usual adjoint, respectively, of the operator $P_t=\exp(At)$ $(t>0)$. Or, by taking its kernel representation, we have

*) The summation convention is not meant, when ε_μ is involved.

$$P(\tilde{x}|\tilde{x}_0;\, t)\rho_0(x_0t) = P(x_0|x;\; t)\rho_0(xt). \tag{5·9}$$

Note that in this representation ρ_0 need not in general be a steady-state solution, but must obey $\partial\rho_0/\partial t = A^+\rho_0 = -\tilde{A}^+\rho_0$.

The above reformulation may be applied readily to the foregoing two examples.

5A. *Master equation (4·1)*

Detailed balance of the 1st kind.

$$W(x'x)\rho_0(x) = W(xx')\rho_0(x'). \tag{5·10}$$

Detailed balance of the 2nd kind.

$$W(\tilde{x}'\tilde{x})\rho_0(xt) = W(xx')\rho_0(x't). \tag{5·11}$$

5B. *Fokker-Planck equation (4·7)*

Detailed balance of the 1st kind.

$$v_{*\mu} = v_\mu = -v_\mu + 2D_{\mu\nu}\frac{\partial}{\partial x_\nu}\log\rho_0 \tag{5·12}$$

which requires

$$\frac{\partial}{\partial x_\nu}(D^{-1}_{\mu\lambda}v_\lambda) = \frac{\partial}{\partial x_\mu}(D^{-1}_{\nu\lambda}v_\lambda). \tag{5·13}$$

This is the simple form of what is called the potential condition, allowing a quadrature for the steady-state solution in the form $\rho_0(x) = \exp(\int^x D^{-1}_{\mu\nu}v_\nu dx_\mu)$.

Detailed balance of the 2nd kind.

$$v_{*\mu} = \tilde{v}_\mu (= \varepsilon_\mu v_\mu(\tilde{x})) = -v_\mu + 2D_{\mu\nu}\frac{\partial\theta}{\partial x_\nu}, \qquad \theta = \log\rho_0\,. \tag{5·14}$$

Thus, the drift velocity can be decomposed into a reversible and an irreversible part, such that $v_\nu = v_\mu{}^{(r)} + v_\mu{}^{(i)}$ and

$$x^{(i)}_\mu \equiv \frac{v_\mu + \tilde{v}_\mu}{2} = D_{\mu\nu}\frac{\partial}{\partial x_\nu}\log\rho_0\,, \tag{5·15}$$

$$v^{(r)}_\mu \equiv \frac{v_\mu - \tilde{v}_\mu}{2}\,. \tag{5·16}$$

These are inserted into Eq. (4·10) to get

$$\frac{\partial\rho_0}{\partial t} + \frac{\partial}{\partial x_\mu}(v^{(r)}_\mu\rho_0) = 0\,. \tag{5·17}$$

Further, the time reversal of the Lagrangian $\tilde{L}$ is compared to $\bar{L}$ in (4·14′), giving the condition for $\tilde{D}_{\mu\nu}$:

$$\tilde{D}_{\mu\nu}(x)\,(= \varepsilon_\mu\varepsilon_\nu D_{\mu\nu}(\tilde{x})) = D_{\mu\nu}(x). \tag{5·18}$$

The argument is the same as given by Graham and Haken.[5] It can be said that

Eqs. (5·15), (5·17) and (5·18) are the necessary and sufficient condition (Graham and Haken's potential condition) for the detailed balance of the second kind to hold in the Fokker-Planck equations (4·7), (4·7′), which in turn may be summarized to say that *the Onsager-Machlup deterministic trajectories are invariant against the time-reversal operation on the dynamical variables.*

We may remark in passing that the detailed balance of the first kind is the strongest among others and, according to Hepp,[9] can be resulted from the assumption of the Gibbs equilibrium states for every infinite reservoirs in the weak coupling treatment of the theory of open systems.

§ 6. Symmetry relations for Markoffian correlation functions

We shall define the standard form of a correlation function in the stationary Markoff process (the generating operator independent of time) in the following:

$$\Phi_{gf}(t) = \int\int f(x_0)\, g(x)\, P(x|x_0;\, t)\, \rho_0(x_0)\, dx_0 dx\,, \tag{6·1}$$

where $P(x|x_0;\, t)$ denotes the transition probability density (from $t=0$ with $x=x_0$ to t) as before, and $\rho_0(x_0)$ the steady state. In order to include the time-reversal symmetry we consider the function to depend on all the external variables which change sign (such as a magnetic field and a Coriolis force) by the time reversal. Denoting them by a single parameter Θ, we write as

$$\Phi_{gf}(t, \Theta) = \int\int f(x_0\Theta)\, g(x\Theta)\, P(x|x_0;\, t\Theta)\, \rho_0(x_0\Theta)\, dx_0 dx\,. \tag{6·2}$$

This expression may be compared with Kubo's (quantum mechanical) correlation function[2]

$$\Phi_{gf}(t, \Theta) \equiv \mathrm{Tr}\, \rho_0 \{ f e^{it\mathcal{H}} g e^{-it\mathcal{H}} \}, \tag{6·3}$$

whose symmetry properties have been summarized by

1) $$\Phi_{gf}(t, \Theta) = \text{real}\,, \tag{6·4}$$

2) $$\Phi_{gf}(-t, \Theta) = \Phi_{fg}(t, \Theta), \tag{6·5}$$

3) $$\Phi_{gf}(t, \Theta) = \varepsilon_f \varepsilon_g \Phi_{gf}(-t, -\Theta) \tag{6·6}$$

$$= \varepsilon_f \varepsilon_g \Phi_{fg}(t, -\Theta). \tag{6·6′}$$

$$(\tilde{f} = \varepsilon_f f\,, \quad \tilde{g} = \varepsilon_g g)$$

It is the microscopic reversibility that makes 3) to be valid; more precisely the right-hand side of the last equality (6·6′) equated to the left-hand side: The process going from Eq. (6·6) to (6·6′) is due to 2) which does not use the reversibility.

We now show that the symmetry property 2) has a universal nature also valid for our Markoffian correlation function defined in (6·2) irrespective of the reversibility. It is a consequence of the relation satisfied between the transition probability density of a process and its time-reversed one in the foregoing general procedure, namely

$$P_*(x_0t_0|xt)\rho_0(xt)=P(xt|x_0t_0)\rho_0(x_0t_0). \tag{6·7}$$

and in particular for the stationary process (for which $t_0=0$ without loss of generality)

$$P_*(x_0|x;-t)\rho_0(x)=P(x|x_0;t)\rho_0(x_0). \tag{6·8}$$

Note that this representation is identical with Eq. (2·16). One can consider the relation in Eq. (6·7) to define a simultaneous interchange of the space-time variables (xt) and (x_0t_0) in the product $P\rho_0$, the transition probability density times a fixed solution density of the evolution equation, so that the subscript $*$ on the left may be dropped. This in fact makes it possible to assign the product $P\rho_0$ as a joint probability density in regard to the two *events* (xt) and (x_0t_0), because it should be symmetric with respect to the interchange of events.

We can now summarize the symmetry relations satisfied by the Markoffian correlation functions $\Phi_{gf}(t,\Theta)$ besides 1) and 2)

3) $$\Phi_{gf}(t,\Theta)=\varepsilon_f\varepsilon_g\Phi_{gf}(-t,-\Theta) \tag{6·9}$$

$$=\varepsilon_f\varepsilon_g\Phi_{fg}(t,-\Theta), \tag{6·9'}$$

(under the detailed balance of the 2nd kind to hold)

3') $$\Phi_{gf}(t,\Theta)=\Phi_{gf}(-t,\Theta) \tag{6·10}$$

$$=\Phi_{fg}(t,\Theta). \tag{6·10'}$$

(under the detailed balance of the 1st kind to hold)

A noticeable point here is that the "irreversible circulation" in Tomita's investigation[6)~8)] pertains to a violation of 3) and 3'), for which, however, 2) still holds and the relation (6·8) gives another representation of what he called "cyclic balance".

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Note added in proof: 1. It is desirable to establish a simpler criterion for this physical concept of "dissipative operator". Recently, Lindblad and also Kishimoto have studied this problem (to be published in Comm. Math. Phys.), obtaining the condition in the form

$$A(f^2)\geq 2fA(f).$$

This can be shown to make the argument in § 3 improved.

2. After this paper was submitted the author has learned the two established stochastic integration schemes viz., "Ito's integral" and "Stratonovich's integral", according to which the OM Lagrangian is differently presented in the path-integration formula. Equation (4·11′) as well as the associated Fokker-Planck equations in 4B are in the scheme of Stratonovich. For a discussion of the most probable path there exists another Lagrangian based on the scheme of Ito. The author is thankful to Dr. H. Nakazawa for his illuminating instruction about this matter.