Progress of Theoretical Physics, Vol. 57, No. 5, May 1977

Thermodynamic Properties of Non-Equilibrium States Subject to Fokker-Planck Equations

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(Received October 18, 1976)

We investigate the relationship between fluctuation theory and thermodynamic theory of non-equilibrium states assuming the Fokker-Planck equation for the evolution law, and deduce two formulas corresponding to the entropy and entropy-production balance equations in thermodynamics

$$\text{I.}\qquad \frac{\partial}{\partial t}\left(-\log\frac{\psi}{\psi_0}\right)\psi+\frac{\partial}{\partial x_\lambda}\left(J_\lambda\left(-\log\frac{\psi}{\psi_0}\right)-V_\lambda\right)\psi=V_\mu X_\mu\psi\geq 0\,,$$

$$\text{II.}\qquad \frac{\partial}{\partial t}(V_\mu X_\mu)\psi+\frac{\partial}{\partial x_\lambda}\left(J_\lambda V_\mu X_\mu-2\frac{\partial V_\lambda}{\partial x_\mu}V_\mu\right)\psi=-2\left(T_{\mu\nu}V_\mu V_\nu+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\right)\psi\leq 0\,.$$

(ψ and ψ_0 are time-dependent and steady-state solutions of the F-P equation. They are also contained in J_λ, V_μ, X_μ and $T_{\mu\nu}$). The inequality in I represents the second law of thermodynamics (ensured automatically by the F-P equation) while that in II the evolution criterion for stability (not automatically ensured) reflecting the Glansdorff-Prigogine theory, and are considered to realize the thermodynamic proposition without recourse to the local-equilibrium assumption. We discuss briefly the laser instability as an example.

§ 1. Introduction

Fokker-Planck equations have been a useful tool in studies of fluctuation phenomena since the physical investigation of the Brownian motion was advanced in early days.[1),2)] It was attempted also with the equations to provide a statistical mechanical framework for the theory of non-equilibrium states so that the pertinent physical law may be formulated; for example, the entropy increase and Onsager's principle.*)

Thus it would be natural to imagine that an intimate relationship might exist between the statistical theory of fluctuations with Fokker-Planck equations and the thermodynamic theory of non-equilibrium states due to Glansdorff and Prigogine.[5),6)] To date, however, little has been analyzed about the relationship. The present paper (together with a forthcoming one) aims to fill this gap: We intend to show that several important concepts in thermodynamics can be incorporated

*) The first important investigation along this direction which we wish to cite is the paper by M. S. Green[3)] who showed the H-theorem and a derivation of the Onsager's reciprocal relations in the framework of Fokker-Planck equations, and the paper by N. Hashitsume[4)] who showed the Onsager's principle (according to his nomination) of variation in some limited case of the equations. (For this see a recent paper by the author.[15)])

into the statistical mechanical framework by means of the Fokker-Planck equations. The concepts of interests are; entropy flow, entropy production, balance equations, stability-instability, and also several types of variational principles. In this paper we discuss these matters except the variational principles for which a more comprehensive treatment is necessary and is deferred to our later paper.[16] Sections 2∼4 are devoted to establishing the two formulas of entropy and entropy-production balance equation. Their thermodynamic significance is discussed in § 5, which is shown to be connected closely with the evolution criterion of Glansdorff and Prigogine[7] and is useful in studies of instability.

In spite of the thermodynamic feature so announced, we must remark here on a difference between the starting point assumed by the ordinary thermodynamics and that by our Fokker-Planck framework. That is, the former requires the so-called "local equilibrium assumption" on the basis of which the entropy concept is introduced similarly to that in thermal equilibrium, whereas in the latter it is discarded and replaced by the explicit use of "ensemble" the probability density of which is made subject to the Fokker-Planck equation. However, this change will make the applicability of thermodynamics unifying. A good example is laser, for which a qualitative discussion is included in § 6.

§ 2. Balance equations

Let us denote a probability density function of the set of n state variables $\{x_\mu\}$ (in the Cartesian coordinate system) by ψ. Then, the Fokker-Planck equation for ψ which we treat throughout this study will be chosen in the form

$$\frac{\partial \psi}{\partial t} = -\frac{\partial}{\partial x_\mu}(v_\mu \psi) + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial \psi}{\partial x_\nu}\right), \tag{2·1}$$

where $D_{\mu\nu}$, a symmetric and positive tensor satisfying

$$D_{\nu\mu} = D_{\mu\nu}\,,\quad D_{\mu\nu}\xi_\mu\xi_\nu \geq 0 \text{ for any real vector } \xi_\mu\,, \tag{2·2}$$

will be designated as the *diffusion tensor*, and v_μ as the *total drift vector*. (In presenting such equations as in the above, we use the usual summation convention such that a doubly repeated index implies the summation with respect to that index.) These are in general functions of $\{x_\mu\}$ and t. It is known[8] that Eq. (1) is a truncation up to second order of a series with derivatives to infinite order, i.e.,

$$\frac{\partial \psi}{\partial t} = \sum_{s=1}^{\infty} \frac{(-1)^s}{s!} \frac{\partial^s}{\partial x_{\mu_1}\cdots\partial x_{\mu_s}}(K_{\mu_1\cdots\mu_s}\psi) \tag{2·3}$$

so that the drift vector and the diffusion tensor are expressed as

$$v_\mu = K_\mu - \frac{1}{2}\frac{\partial K_{\mu\nu}}{\partial x_\nu} \tag{2·4}$$

and

$$D_{\mu\nu}=\frac{1}{2}K_{\mu\nu}\,. \tag{2·5}$$

As is known from the theory of stochastic processes,[9] the coefficients K's are related to the conditional expectation of the Wiener process as follows:

$$K_{\mu}(\boldsymbol{x})=\lim_{\Delta t\downarrow 0}\left\langle \frac{x_{\mu}(t+\Delta t)-x_{\mu}(t)}{\Delta t}\,\middle|\, x_{\lambda}(t)=x_{\lambda}\right\rangle, \tag{2·6}$$

$$K_{\mu\nu}(\boldsymbol{x})=\lim_{\Delta t\downarrow 0}\left\langle \frac{(x_{\mu}(t+\Delta t)-x_{\mu}(t))\,(x_{\nu}(t+\Delta t)-x_{\nu}(t))}{\Delta t}\,\middle|\, x_{\lambda}(t)=x_{\lambda}\right\rangle. \tag{2·7}$$

It is notable that the mean forward derivative $K_{\mu}(\boldsymbol{x})$ which arises in the corresponding Langevin equation for a Brownian motion $\boldsymbol{B}(\boldsymbol{x}(t))$ in

$$dx_{\mu}=K_{\mu}(\boldsymbol{x})\,dt+dB_{\mu} \tag{2·8}$$

as its mean velocity is generally unequal to the total drift $v_{\mu}(\boldsymbol{x})$, but is related to the latter as Eq. (2·4). The writing of a Fokker-Planck equation in the form (2·1) (which retains the diffusion part as self-adjoint) is not just for the purpose of convenience but for the physical significance of the total drift v_{μ} in many respects.*) Note that the adjoint manipulation associated with the spatial differential operations on ψ is possible only under the satisfaction of the boundary condition for ψ: That is, the probability density function $\psi(\boldsymbol{x}\,t)$ must be rapidly decreasing for $|x|\to\infty$ (the *natural boundary condition* according to Graham[8]) which we assume throughout.

Let us rewrite the Fokker-Planck equation (2·1) in the form of equation of continuity, and consider its effect on any quantity M represented as a function of the space-time variables:

$$\frac{\partial\psi}{\partial t}+\frac{\partial}{\partial x_{\mu}}(J_{\mu}\psi)=0\,. \tag{2·9}$$

We may write an equation involving $M\psi$, by virtue of Eq. (2·9), as

$$\frac{\partial}{\partial t}(M\psi)+\frac{\partial}{\partial x_{\mu}}(J_{\mu}M\psi)=\left(\frac{\partial M}{\partial t}+J_{\mu}\frac{\partial M}{\partial x_{\mu}}\right)\psi\,. \tag{2·10}$$

Here, the current vector J_{μ} which continues ψ may be obtained from Eq. (2·1) as

$$J_{\mu}=v_{\mu}-D_{\mu\nu}\frac{\partial}{\partial x_{\nu}}\log\psi\,, \tag{2·11}$$

showing that the current vector is linearly dependent on $\log\psi$; a fact which is specific to the Fokker-Planck equations. Equation (2·10) represents the local time variation of the density associated with M which consists of two origins;

*) This conforms to a description by R. Graham in a recent article,[8'] where he changed the notation of the total drift (the present v_{μ}) to K_{μ}.

viz., the divergence term $-(\partial/\partial x_\mu)(J_\mu M\psi)$ and the source term $((\partial M/\partial t)+J_\mu \times(\partial M/\partial x_\mu))\psi$. Thus, it corresponds to the *balance equation* associated with the quantity M in thermodynamic theory of irreversible processes.[6] (Here, the probability density ψ replaces the mass density of a constituent substance, and the space of the state variables (i.e., the phase space) by which the F-P equation is written replaces the real space.) It is more clearly demonstrated as follows:

$$\frac{d}{dt}\int_\Omega M\psi d\boldsymbol{x}=\int_{\partial\Omega} M\psi J_\mu d\sigma_\mu(\boldsymbol{x})+\int_\Omega\left(\frac{\partial M}{\partial t}+J_\mu\frac{\partial M}{\partial x_\mu}\right)\psi d\boldsymbol{x}\,, \tag{2·12}$$

where the two kinds of the integration are specified by the volume element dx and the μ-th normal component of the surface element $d\sigma_\mu(\boldsymbol{x})$ of a region Ω whose boundary, $\partial\Omega$, is a smooth surface of Ω. On the right-hand side of (2·12) the first surface integral represents the contribution to M in Ω flowing from outside and the second volume integral that produces within Ω itself. The natural boundary condition on ψ ensures that the integral on the whole space (denoted by R^n) makes the flow contribution to vanish, so that

$$\frac{d}{dt}\int_{R^n} M\psi d\boldsymbol{x}=\int_{R^n}\left(\frac{\partial M}{\partial t}+J_\mu\frac{\partial M}{\partial x_\mu}\right)\psi d\boldsymbol{x}\,. \tag{2·13}$$

§ 3. Entropy and entropy production

The notion "entropy production" is a basic one in thermodynamics of irreversible processes, which we wish to formulate from the present standpoint. Here we assume that the diffusion process described by the Fokker-Planck equation (2·1) is *stationary* by requiring the coefficient functions v_μ and $D_{\mu\nu}$ to be all time-independent. We also assume the existence of a steady-state distribution ψ_0 which satisfies

$$0=-\frac{\partial}{\partial x_\mu}(v_\mu\psi_0)+\frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial\psi_0}{\partial x_\nu}\right) \tag{3·1}$$

under the natural boundary condition. This may impose some further restrictions on the nature of the total drift v_μ and the diffusion coefficients $D_{\mu\nu}$, which we will discuss later to an extent of the stability consideration.

Entropy is a curious quantity since Boltzmann, Gibbs, Ehrenfest and Shannon.*) Concerning the Fokker-Planck equations (2·1) and (3·1), the natural definition of the entropy functional of the distribution ψ relative to ψ_0 is the following integral:

*) We will not go into the historical problem of how to define the entropy in non-equilibrium states.[10] Our standpoint is, however, that as far as concerning Fokker-Planck equations the adoption of the Gibbs entropy functional could provide a far-reaching understanding of thermodynamics. Note that De Groot and Mazur[6] used the same Gibbs functional to discuss the entropy balance equation set up in the coordinate space. The present formulation extends their treatment to the whole phase space.

$$\mathcal{S}\{\psi, \psi_0\} = -\int \left(\log \frac{\psi}{\psi_0}\right)\psi d\boldsymbol{x} \,. \tag{3·2}$$

This is under the normalization condition

$$\int \psi d\boldsymbol{x} = \int \psi_0 d\boldsymbol{x} = 1 \,, \tag{3·3}$$

which are ensured by the respective Fokker-Planck equations. This suggests to introduce the *entropy* for the present purpose as a space-time function $M(\boldsymbol{x}\, t)$ whose balance equation is to be sought:

$$M = -\log \frac{\psi}{\psi_0} \,. \tag{3·4}$$

Our first theorem, then, is expressed by the formula which corresponds to the *entropy balance* in thermodynamics as follows:

$$\frac{\partial}{\partial t}\left(-\log \frac{\psi}{\psi_0}\right)\psi + \frac{\partial}{\partial x_\lambda}\left(J_\lambda\left(-\log \frac{\psi}{\psi_0}\right) - V_\lambda\right)\psi = V_\mu X_\mu \psi \,, \tag{3·5}$$

where

$$X_\mu \equiv \frac{\partial}{\partial x_\mu}\left(-\log \frac{\psi}{\psi_0}\right), \tag{3·5a}$$

$$V_\mu \equiv D_{\mu\nu} X_\nu = D_{\mu\nu} \frac{\partial}{\partial x_\nu}\left(-\log \frac{\psi}{\psi_0}\right), \tag{3·5b}$$

and regarding the current vector introduced in (2·16)

$$J_\mu = v_\mu - v_\mu{}^0 + V_\mu \,, \quad v_\mu{}^0 \equiv D_{\mu\nu} \frac{\partial}{\partial x_\nu} \log \psi_0 \,. \tag{3·5c}$$

We have arranged this formula together with several defining equalities so that it may preserve a formal analogy to the usual thermodynamic version of the entropy balance. That is, the divergence-characteristic term of the entropy flow $J_\lambda(-\log(\psi/\psi_0))\psi$ plus the extra one $-V_\lambda\psi$ on the left-hand side and a term bilinear in regards to the two vectors X_μ and V_μ defined in Eqs. (3·5a) and (3·5b), respectively, on the right-hand side of Eq. (3·5). Evidently, the vector X_μ corresponds to the (generalized) *force* and V_μ to the *flux*, although in the present version these quantities contain the instantaneous distribution $\psi(\boldsymbol{x}\, t)$; a basically different feature from what the ordinary thermodynamics indicates. The point of implication of formula (3·4) is that the removal of the local equilibrium assumption in the ordinary theory still enables one to maintain its essence of the assertion of entropy balance written in the phase space in the present Fokker-Planck framework, provided the entropy density is so defined as to conform to the Gibbs functional.

Thus, in view of the right-hand expression of Eq. (3·5), we designate the

quantity $V_\mu X_\mu$ as the *entropy production* in the present framework. It is then interesting to inquire the balance equation associated with this quantity in connection with the work of Glansdorff and Prigogine.[5] Our second theorem is to answer to this inquiry, and is expressed as follows:

$$\frac{\partial}{\partial t}(V_\mu X_\mu)\psi+\frac{\partial}{\partial x_\lambda}\left(J_\lambda V_\mu X_\mu-2\frac{\partial V_\lambda}{\partial x_\mu}V_\mu\right)\psi$$

$$=-2\left(T_{\mu\nu}V_\mu V_\nu+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\right)\psi\,, \tag{3·6}$$

where the tensor $T_{\mu\nu}$, designated as the stress tensor, is given by

$$T_{\mu\nu}=-\frac{\partial}{\partial x_\nu}(D^{-1}_{\mu\lambda}v_\lambda{}^0)+D^{-1}_{\mu\lambda}\frac{\partial}{\partial x_\nu}(v_\lambda-v_\lambda{}^0)+\frac{1}{2}J_\lambda\frac{\partial D^{-1}_{\mu\nu}}{\partial x_\lambda} \tag{3·6a}$$

in which D^{-1} is the inverse tensor of $D(D^{-1}_{\mu\lambda}D_{\lambda\nu}=\delta_{\mu\nu})$ and $v_\lambda{}^0$ is defined in Eq. (3·5c). We will show the derivation of the two formulas (3·5) and (3·6) and discuss their physical significance separately in the following sections. Here we note a simplification of the expression (3·6a) under the satisfaction of the *potential condition*.[8),11)]

If there exists a set of symmetry relations among the n components of the vector $(D^{-1}v)_\mu=D^{-1}_{\mu\lambda}v_\lambda$

$$\frac{\partial}{\partial x_\nu}(D^{-1}_{\mu\lambda}v_\lambda)=\frac{\partial}{\partial x_\mu}(D^{-1}_{\nu\lambda}v_\lambda)\,, \tag{3·7}$$

then the differential form $-D^{-1}_{\mu\lambda}v_\lambda dx_\mu$ is the total differential of a scalar function denoted by ϕ so that

$$d\phi=-D^{-1}_{\mu\lambda}v_\lambda dx_\mu\,. \tag{3·8}$$

It satisfies

$$D_{\mu\nu}\frac{\partial\phi}{\partial x_\nu}=-v_\mu$$

and, by setting $-(\partial\phi/\partial x_\mu)=(1/\psi_0)(\partial\psi_0/\partial x_\mu)$, is equivalent to

$$-v_\mu\psi_0+D_{\mu\nu}\frac{\partial\psi_0}{\partial x_\nu}=0\,,$$

reducing to the Fokker-Planck equation for the steady-state (3·1). This is the simplest case of the potential condition[11] for which the steady-state distribution ψ_0 is given by

$$\psi_0=e^{-\phi} \tag{3·9}$$

$$=\exp\left(\int^x D^{-1}_{\mu\nu}v_\nu dx_\mu+\text{const}\right). \tag{3·9a}$$

Under this circumstance

$$v_\lambda^0 = v_\lambda\,,\quad J_\lambda = V_\lambda = D_{\lambda\mu}X_\mu\,, \tag{3·10}$$

and the stress tensor $T_{\mu\nu}$ becomes symmetric and is simplified to

$$T_{\mu\nu}(=T_{\nu\mu}) = \frac{\partial^2\phi}{\partial x_\mu \partial x_\nu} + \frac{1}{2}\,V_\lambda \frac{\partial D_{\mu\nu}^{-1}}{\partial x_\lambda}\,, \tag{3·6a′}$$

indicating that the principal part of the stress tensor comes from the second-order derivative tensor of the potential ϕ. Such an exposition of the tensor $T_{\mu\nu}$ is, however, always possible (even in the absence of the simplest potential condition as above), if the steady-state distribution ψ_0 is represented in terms of the potential as in (3·9) (thereby (3·9a) may not hold), so that

$$T_{\mu\nu} = \frac{\partial^2\phi}{\partial x_\mu \partial x_\nu} + \frac{1}{2}\,J_\lambda \frac{\partial D_{\mu\nu}^{-1}}{\partial x_\lambda} + D_{\mu\lambda}^{-1}\frac{\partial}{\partial x_\nu}(v_\lambda - v_\lambda^0)\,. \tag{3·6a″}$$

(Under general circumstances the tensor $T_{\mu\nu}$ given by (3·6a″) may not be symmetric, the asymmetric part coming from the third term on the right. Note that the antisymmetric part of $T_{\mu\nu}$ is irrelevant to the balance equation (3·6).)

§ 4. Detailed derivation of the two balance equations

Derivation of the entropy balance equation (3·5)

Let us put $M = \log(\psi/\psi_0)$, where ψ and ψ_0 are time-dependent and a steady-state solution of the Fokker-Planck equation, respectively, and obtain the right-hand side of the balance equation for M. For this purpose it is convenient to rewrite the respective Fokker-Planck equations in the form

$$\frac{\partial}{\partial t}\log\psi + (v_\lambda - v_\lambda^0 + V_\lambda)\frac{\partial}{\partial x_\lambda}\log\psi + \frac{\partial}{\partial x_\lambda}(v_\lambda - v_\lambda^0 + V_\lambda) = 0\,, \tag{4·1}$$

$$(v_\lambda - v_\lambda^0)\frac{\partial}{\partial x_\lambda}\log\psi_0 + \frac{\partial}{\partial x_\lambda}(v_\lambda - v_\lambda^0) = 0\,, \tag{4·2}$$

i.e., the evolution equations pertaining to the *logarithm* of the probability densities. The two velocity-vectors V_λ and v_λ^0 are the same as defined before, i.e.,

$$V_\lambda = D_{\lambda\nu}\frac{\partial}{\partial x_\nu}\left(-\log\frac{\psi}{\psi_0}\right),\quad v_\lambda^0 = D_{\lambda\nu}\frac{\partial}{\partial x_\nu}\log\psi_0\,. \tag{4·3}$$

A subtraction of Eq. (4·2) from (4·1) on both sides yields

$$\frac{\partial}{\partial t}\log\frac{\psi}{\psi_0} + J_\lambda\frac{\partial}{\partial x_\lambda}\log\frac{\psi}{\psi_0} = -V_\lambda\frac{\partial}{\partial x_\lambda}\log\psi_0 - \frac{\partial}{\partial x_\lambda}V_\lambda\,. \tag{4·4}$$

By multiplying both sides of Eq. (4·4) by ψ, we get

$$\left(\frac{\partial}{\partial t}\log\frac{\psi}{\psi_0} + J_\lambda\frac{\partial}{\partial x_\lambda}\log\frac{\psi}{\psi_0}\right)\psi = \left(-\frac{\partial}{\partial x_\lambda}V_\lambda\right)\psi - \left(V_\lambda\frac{\partial}{\partial x_\lambda}\log\psi_0\right)\psi$$

$$= -\frac{\partial}{\partial x_\lambda}(V_\lambda\psi) + V_\lambda\frac{\partial\psi}{\partial x_\lambda} - \left(V_\lambda\frac{\partial}{\partial x_\lambda}\log\psi_0\right)\psi$$

$$= -\frac{\partial}{\partial x_\lambda}(V_\lambda\psi) + V_\lambda\left(\frac{\partial}{\partial x_\lambda}\log\frac{\psi}{\psi_0}\right)\psi\,. \tag{4·5}$$

This last expression is inserted into the right-hand side of the balance equation, leading us to write Eq. (2·15) for $M=\log(\psi/\psi_0)$ as

$$\frac{\partial}{\partial t}\left(\log\frac{\psi}{\psi_0}\right)\psi + \frac{\partial}{\partial x_\lambda}\left(J_\lambda\left(\log\frac{\psi}{\psi_0}\right)\psi\right) = -\frac{\partial}{\partial x_\lambda}(V_\lambda\psi) + V_\lambda\left(\frac{\partial}{\partial x_\lambda}\log\frac{\psi}{\psi_0}\right)\psi\,.$$

The first term on the right-hand side may be transferred to the left and incorporated into the divergence term. Consequently, introducing the "force"

$$X_\mu = \frac{\partial}{\partial x_\mu}\left(-\log\frac{\psi}{\psi_0}\right) \text{ (so that } V_\mu = D_{\mu\nu}X_\nu), \tag{4·6}$$

and making a sign-reverse, we obtain the result

$$\frac{\partial}{\partial t}\left(-\log\frac{\psi}{\psi_0}\right)\psi + \frac{\partial}{\partial x_\lambda}\left(J_\lambda\left(-\log\frac{\psi}{\psi_0}\right) - V_\lambda\right)\psi = V_\mu X_\mu\psi\,. \tag{4·7}$$

Derivation of the entropy-production balance equation (3·6)

We put $M=V_\mu X_\mu$ as before, where X_μ and V_μ are defined in (3·5a) and (3·5b) (also in (4·6) and (4·3)). Then, to deduce the right-hand side of the balance equation (3·6), we begin with the following manipulation:

$$\frac{\partial}{\partial t}(V_\mu X_\mu) + J_\lambda\frac{\partial}{\partial x_\lambda}(V_\mu X_\mu)$$

$$= V_\mu\left(\frac{\partial X_\mu}{\partial t} + J_\lambda\frac{\partial X_\mu}{\partial x_\lambda}\right) + \left(\frac{\partial V_\mu}{\partial t} + J_\lambda\frac{\partial V_\mu}{\partial x_\lambda}\right)X_\mu$$

$$= D_{\mu\nu}X_\nu\left(\frac{\partial X_\mu}{\partial t} + J_\lambda\frac{\partial X_\mu}{\partial x_\lambda}\right) + D_{\mu\nu}\left(\frac{\partial X_\nu}{\partial t} + J_\lambda\frac{\partial X_\nu}{\partial x_\lambda}\right)X_\mu$$

$$+ J_\lambda\frac{\partial D_{\mu\nu}}{\partial x_\lambda}X_\mu X_\nu$$

$$= 2V_\nu\left(\frac{\partial X_\nu}{\partial t} + J_\lambda\frac{\partial X_\nu}{\partial x_\lambda}\right) + J_\lambda\frac{\partial D_{\mu\nu}}{\partial x_\lambda}D^{-1}_{\mu\mu'}D^{-1}_{\nu\nu'}V_{\mu'}V_{\nu'}\,.$$

In the last expression we may use the relation

$$\frac{\partial D_{\mu\nu}}{\partial x_\lambda}D^{-1}_{\mu\mu'}D^{-1}_{\nu\nu'} = -\frac{\partial D^{-1}_{\mu'\nu'}}{\partial x_\lambda} \tag{4·8}$$

as a consequence of the derivation of the identity $D_{\mu\nu}D^{-1}_{\nu\nu'}=\delta_{\mu\nu'}$, so that we have

$$\frac{\partial}{\partial t}(V_\mu X_\mu) + J_\lambda\frac{\partial}{\partial x_\lambda}(V_\mu X_\mu)$$

$$=2V_\nu\left(\frac{\partial X_\nu}{\partial t}+J_\lambda\frac{\partial X_\nu}{\partial x_\lambda}\right)-J_\lambda\frac{\partial D^{-1}_{\mu\nu}}{\partial x_\lambda}V_\mu V_\nu\,. \tag{4·9}$$

Thus the problem reduces to reexpressing $(\partial X_\nu/\partial t)+J_\lambda(\partial X_\nu/\partial x_\lambda)$ in terms of V_μ, $\partial V_\mu/\partial x_\nu$ etc., for which our previous result may be aided.

Let us recall Eq. (4·4), i.e.,

$$\frac{\partial}{\partial t}\log\frac{\psi}{\psi_0}+J_\lambda\frac{\partial}{\partial x_\lambda}\log\frac{\psi}{\psi_0}=-V_\lambda\frac{\partial}{\partial x_\lambda}\log\psi_0-\frac{\partial}{\partial x_\lambda}V_\lambda\,, \tag{4·10}$$

where

$$J_\lambda=v_\lambda-v_\lambda^0+V_\lambda\,. \tag{4·10a}$$

We apply the differential operation $-(\partial/\partial x_\nu)$ on both sides of Eq. (4·10), writing

$$\frac{\partial}{\partial t}\frac{\partial}{\partial x_\nu}\left(-\log\frac{\psi}{\psi_0}\right)+J_\lambda\frac{\partial^2}{\partial x_\lambda\partial x_\nu}\left(-\log\frac{\psi}{\psi_0}\right)+\frac{\partial J_\lambda}{\partial x_\nu}\frac{\partial}{\partial x_\lambda}\left(-\log\frac{\psi}{\psi_0}\right)$$
$$=\frac{\partial}{\partial x_\nu}\left(V_\lambda\frac{\partial}{\partial x_\lambda}\log\psi_0\right)+\frac{\partial^2 V_\lambda}{\partial x_\lambda\partial x_\nu}\,. \tag{4·11}$$

The last term on the left-hand side of Eq. (4·11) may be transferred to the right, and by virtue of the definition of the "force" in (4·6), Eq. (4·11) is rewritten as

$$\frac{\partial X_\nu}{\partial t}+J_\lambda\frac{\partial X_\nu}{\partial x_\lambda}=\frac{\partial}{\partial x_\nu}\left(V_\lambda\frac{\partial}{\partial x_\lambda}\log\psi_0\right)-\frac{\partial J_\lambda}{\partial x_\nu}X_\lambda+\frac{\partial^2 X_\lambda}{\partial x_\lambda\partial x_\nu}$$
$$=\frac{\partial}{\partial x_\nu}\left(V_\mu\frac{\partial}{\partial x_\mu}\log\psi_0\right)-\frac{\partial V_\lambda}{\partial x_\nu}X_\lambda$$
$$-\frac{\partial(v_\lambda-v_\lambda^0)}{\partial x_\nu}X_\lambda+\frac{\partial^2 V_\lambda}{\partial x_\lambda\partial x_\nu}$$
$$=\frac{\partial}{\partial x_\nu}\left(V_\mu\frac{\partial}{\partial x_\mu}\log\psi_0\right)-\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial}{\partial x_\mu}\log\psi_0$$
$$-D^{-1}_{\mu\lambda}\frac{\partial(v_\lambda-v_\lambda^0)}{\partial x_\nu}V_\mu$$
$$+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial}{\partial x_\mu}\log\psi+\frac{\partial^2 V_\mu}{\partial x_\mu\partial x_\nu}\,. \tag{4·12}$$

(A use of Eqs. (4·10a), (4·6) and a change of running index have been made.) This last expression is readily simplified, by regrouping the 1st and 2nd and also 4th and 5th terms on the right-hand side of (4·12), so that

$$\frac{\partial X_\nu}{\partial t}+J_\lambda\frac{\partial X_\nu}{\partial x_\lambda}=\left(\frac{\partial}{\partial x_\nu}(D^{-1}_{\mu\lambda}v_\lambda^0)-D^{-1}_{\mu\lambda}\frac{\partial(v_\lambda-v_\lambda^0)}{\partial x_\nu}\right)V_\mu$$
$$+\frac{1}{\psi}\frac{\partial}{\partial x_\mu}\left(\psi\frac{\partial V_\mu}{\partial x_\nu}\right) \tag{4·13}$$

which can be inserted into Eq. (4·9). The result is

$$\frac{\partial}{\partial t}(V_\mu X_\mu)+J_\lambda\frac{\partial}{\partial x_\lambda}(V_\mu X_\mu)$$
$$=-2T_{\mu\nu}V_\mu V_\nu+\frac{2}{\psi}V_\nu\frac{\partial}{\partial x_\mu}\left(\psi\frac{\partial V_\mu}{\partial x_\nu}\right), \tag{4·14}$$

where

$$T_{\mu\nu}=-\frac{\partial}{\partial x_\nu}(D^{-1}_{\mu\lambda}v_\lambda{}^0)+D^{-1}_{\mu\lambda}\frac{\partial}{\partial x_\nu}(v_\lambda-v_\lambda{}^0)+\frac{1}{2}J_\lambda\frac{\partial D^{-1}_{\mu\nu}}{\partial x_\lambda}. \tag{4·14a}$$

Finally, in terms of this stress tensor $T_{\mu\nu}$ the entropy-production balance equation is obtained through a procedure just the same as before (from (4·4) to (4·7)) in the form

$$\frac{\partial}{\partial t}(V_\mu X_\mu\psi)+\frac{\partial}{\partial x_\lambda}\left(J_\lambda V_\mu X_\mu-2\frac{\partial V_\lambda}{\partial x_\mu}V_\mu\right)\psi$$
$$=-2\left(T_{\mu\nu}V_\mu V_\nu+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\right)\psi. \tag{4·15}$$

§ 5. The second law of thermodynamics and the stability problem

Consider first the entropy balance equation (3·5):

I. $$\frac{\partial}{\partial t}\left(-\log\frac{\psi}{\psi_0}\right)\psi+\frac{\partial}{\partial x_\lambda}\left(J_\lambda\left(-\log\frac{\psi}{\psi_0}\right)-V_\lambda\right)\psi=V_\mu X_\mu\psi.$$

The right-hand side of this formula may be designated as the entropy production density in accordance with the argument in § 3, for which by virtue of (2·2) and (3·5b)

$$V_\mu X_\mu\psi=D_{\mu\nu}X_\mu X_\nu\psi\geq 0, \tag{5·1}$$

indicating that the entropy production is always positive. Formula I with the inequality (5·1) is a local representation of the second law of thermodynamics. For, an integration over the whole space of both sides of I yields the well-known H-theorem[3),12)]

$$\frac{d}{dt}\int_{R^n}\left(-\log\frac{\psi}{\psi_0}\right)\psi dx=\int_{R^n}D_{\mu\nu}\left(\frac{\partial}{\partial x_\mu}\log\frac{\psi}{\psi_0}\right)\left(\frac{\partial}{\partial x_\nu}\log\frac{\psi}{\psi_0}\right)\psi d\boldsymbol{x}.$$
$$\geq 0. \tag{5·2}$$

As to a restricted region Ω, the integration shows that the entropy change comes from two origins:

$$\frac{d}{dt}\int_\Omega\left(-\log\frac{\psi}{\psi_0}\right)\psi d\boldsymbol{x}=\int_{\partial\Omega}\left(J_\lambda\left(-\log\frac{\psi}{\psi_0}\right)-V_\lambda\right)\psi d\sigma_\lambda(\boldsymbol{x})$$

$$+\int_{\Omega} D_{\mu\nu}\left(\frac{\partial}{\partial x_\mu}\log\frac{\psi}{\psi_0}\right)\left(\frac{\partial}{\partial x_\nu}\log\frac{\psi}{\psi_0}\right)\psi d\boldsymbol{x}\,, \qquad (5\cdot3)$$

viz., the production contribution inside of the region (≥ 0) and the flow contribution through the boundary $\partial\Omega$, the latter sign being not definite. Consequently, the left-hand side of Eq. (5·3) may be of negative sign, if the flow contribution exceeds negatively the internal production. Such is the case, as we will discuss in § 6, if an instability takes place.

Next, we discuss the entropy-production balance equation (3·6):

II.
$$\frac{\partial}{\partial t}(V_\mu X_\mu\psi)+\frac{\partial}{\partial x_\lambda}\left(J_\lambda V_\mu X_\mu-2\frac{\partial V_\lambda}{\partial x_\mu}V_\mu\right)\psi$$
$$=-2\left(T_{\mu\nu}V_\mu V_\nu+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\right)\psi\,.$$

The thermodynamic theory of the Glansdorff-Prigogine states that the time derivative of the entropy production should be of negative sign for a stable evolution of the system. This is based on the consideration that the increase of entropy by the second law must be more gradual when the system approaches the equilibrium position (linked with the principle of minimum entropy production), which has been proved near-equilibrium situation and extended to far from equilibrium.[7),*)] This criterion of evolution suggests that in the present Fokker-Planck framework one puts a negative sign on the right-hand side of formula II, so that

$$\left(T_{\mu\nu}V_\mu V_\nu+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\right)\psi\geq 0\,. \qquad (5\cdot4)$$

Unlike the second law inequality (5·1), this inequality is not verifiable from the Fokker-Planck equation (2·1) in itself: One has always

$$\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\geq 0\,, \qquad (5\cdot5)$$

but $T_{\mu\nu}$ is not necessarily a positive tensor.

As we have discussed in the end of § 3, the stress tensor $T_{\mu\nu}$ is expressed in terms of the potential $\phi=-\log\psi_0$ as

*) The statement may be interpreted in the present notation by

$$\int V_\mu\frac{\partial X_\mu}{\partial t}\psi d\boldsymbol{x}\leq 0 \qquad (A)$$

but not in the form expressed as the total time-derivative as in formula II. In view of this, we examine the validity of this inequality in the present framework. A mainipulation similar to § 4 gives

$$\int V_\mu\frac{\partial X_\mu}{\partial t}\psi\, d\boldsymbol{x}=-\int(v_\lambda-v_\lambda^0)X_\lambda\frac{\partial(V_\mu\psi)}{\partial x_\mu}d\boldsymbol{x}-\int\left(\frac{\partial}{\partial x_\mu}(V_\mu\psi)\right)^2\frac{1}{\psi}d\boldsymbol{x}\,. \qquad (B)$$

This shows that the potential condition (3·7) and hence (3·10) ensures the inequality $\int V_\mu(\partial X_\mu/\partial t)\cdot\psi d\boldsymbol{x}\leq 0$, but otherwise (A) is generally not true.

$$T_{\mu\nu}=\frac{\partial^2\phi}{\partial x_\mu\partial x_\nu}+\frac{1}{2}J_\lambda\frac{\partial D^{-1}_{\mu\nu}}{\partial x_\lambda}+D^{-1}_{\mu\nu}\frac{\partial}{\partial x_\nu}(v_\lambda-v_\lambda{}^0). \tag{5·6}$$

Generally, the second-order derivative tensor $(\partial^2/\partial x_\mu\partial x_\nu)\phi$ dominates over the other terms (which is true at least under the potential condition and the constant diffusion tensor), and

$$\frac{\partial^2\phi}{\partial x_\mu\partial x_\nu}\xi_\mu\xi_\nu\geq 0 \quad \text{for} \quad |\boldsymbol{x}|\to\infty \tag{5·7}$$

because of the assumption that the steady-state distribution ψ_0 exists satisfying the natural boundary condition. Thus inequality (5·4) holds provided the deterministic motion by the potential ϕ is stable. It is an instability of the motion that the evolution criterion (5·4) becomes critical, where the left-hand side consists of the two competing quantities; one negative due to the unstable motion and the other positive which represents the effect of fluctuations relaxing the former. The Fokker-Planck equation therefore establishes a representation of the Glansdorff-Prigogine criterion of evolution in the form of competition between the organization and the randomness and the prediction of the latter to overcome the former for the over all stability.

Remark The inequality of stability evolution criterion in II is a proposition which has not been established with a general proof, as mentioned above. It is interesting, therefore, to discover its condition of validity. One conjectures that the existence of the solutions ψ and ψ_0 is sufficient for it. It is highly desirable to ascertain whether it is true or not.

§ 6. Application to laser instability

The best example to which the foregoing formulation may apply is the single-mode laser action which has been studied extensively by using a Fokker-Planck equation.[13] We reconsider the problem qualitatively from the present thermodynamic point of view.*) The laser Fokker-Planck equation may be written (after the elimination of an atomic freedom) as

$$\frac{\partial\psi}{\partial t}=-\left(\frac{\partial}{\partial x}v_x\psi+\frac{\partial}{\partial y}v_y\psi\right)+D\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right), \tag{6·1}$$

$$D=\text{const}, \tag{6·1a}$$

$$v_x(x,y)=D(a-a_2r^2)x\,,\quad v_y(x,y)=D(a-a_2r^2)y \tag{6·1b}$$

which satisfies the potential condition, so that

*) A unification of the laser theory in a macroscopic standpoint and the Glansdorff-Prigogine theory has been discussed by R. Graham,[14] who pointed out some difficulty in associating the concepts of both entropy and entropy production with quantities to be derived from the single potential function ϕ, proposing a counter consideration. Our formulation should answer to his questioning, which will be discussed elsewhere together with a full numerical analysis. (Note added in proof)

$$\phi(x, y) = -\frac{a}{2} r^2 + \frac{a_2}{4} r^4, \quad r = \sqrt{x^2 + y^2}, \tag{6·2}$$

$$v_x = -D \frac{\partial \phi}{\partial x}, \quad v_y = -D \frac{\partial \phi}{\partial y} \tag{6·3}$$

and

$$\psi_0(x, y) \ (\equiv \psi_0(r)) = N e^{-\phi(x, y)}. \tag{6·4}$$

The natural boundary condition requires that the constant a_2 must be positive while the other one a, the pumping parameter, may vary from $-\infty$ to $+\infty$, but the situation

$$a \gg \sqrt{a_2} \tag{6·5}$$

is of particular interest which corresponds to far above threshold.

In the situation of (6·5), the potential ϕ is of the form such that its minimum points encircles the origin of the x-y plane, i.e., the complex plane of the active mode amplitude. These minima yield the stable equilibrium of the deterministic motion

$$\dot{x} = v_x, \quad \dot{y} = v_y, \tag{6·6}$$

and corresponds to the state of steady photon generation, while the origin, the 0-photon state, yields the unique unstable equilibrium. It is the most interesting feature of a transient laser action that the initial distribution peaked at the 0-photon state undergoes flattening, not to reach a completely broadened distribution, but to reach the steady-state distribution ψ_0 peaked at around the minimum circle of ϕ, the appearance of this peak being considered as a kind of the "dissipative structure" formation.[14]

The disappearance of the 0-photon peak at the initial stage may be considered as a consequence of the entropy production accompanied by the dissipative time-evolution of the states. Actually, it is not a mere dissipation, the instability of the motion (6·6) enhancing the "fall". The effect of this enhancement can be seen from the entropy production balance equation II as follows:

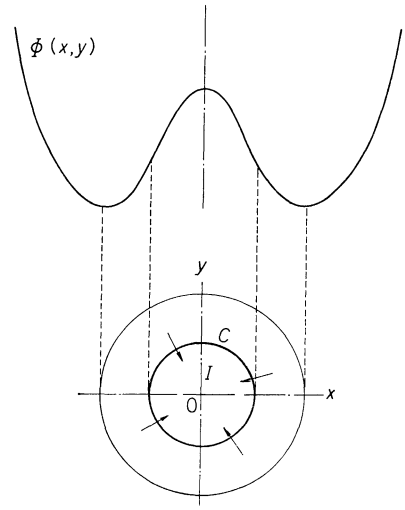

Fig. 1. The instability region (denoted by I) which is surrounded by the instability circle (denoted by C) in the complex plane of the active mode amplitude in the laser action. The arrows indicate a systematic entropy flow to cause the "grow" of the steady state distribution.

$$\frac{\partial}{\partial t}(V_\mu X_\mu)\psi+\frac{\partial}{\partial x_\lambda}\left(J_\lambda V_\mu X_\mu-2\frac{\partial V_\lambda}{\partial x_\mu}V_\mu\right)\psi$$
$$=-2\left(T_{\mu\nu}V_\mu V_\nu+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\right)\psi\,,\quad \lambda,\mu,\nu=x \text{ and } y$$

where

$$T_{\mu\nu}=\frac{\partial^2\phi}{\partial x_\mu\partial x_\nu} \tag{6·7}$$

by virtue of the potential condition and of the constancy of the diffusion coefficient. Let us call the region where $T_{\mu\nu}\xi_\mu\xi_\nu\leq 0$ the *instability region*. For the function ϕ given in (6·2) it is the inside of a circle C specified by

$$C:\ \frac{d^2\phi}{dr^2}=0 \text{ inside of which } \frac{d^2\phi}{dr^2}<0\,, \tag{6·8}$$

which is located inside the minimum circle. (Fig. 1) Thus, on the right-hand side of the formula II the two terms $T_{\mu\nu}V_\mu V_\nu$ and $(\partial V_\mu/\partial x_\nu)(\partial V_\nu/\partial x_\mu)$ are competing each other, implying that the increase of entropy by the second law is hardly suppressed in the instability region. In this sense, the instability of the deterministic motion is *against* the evolution criterion (as it should). The second term $(\partial V_\mu/\partial x_\nu)(\partial V_\nu/\partial x_\mu)$ which arises due to fluctuations moderates the negative value of the first term $(\partial^2\phi/\partial x_\mu\partial x_\nu)V_\mu V_\nu$ to recover the evolution criterion generally. (This is a feature of the present formulation to remedy the inadequacy[14] of the theory which identifies $-\phi(\boldsymbol{x})=\log\psi_0(\boldsymbol{x})$ with the entropy to be applied to the Glansdorff-Prigogine theory.)

The enhancement of the entropy increase at around the instability region should be linked with a "grow" of the distribution ψ outside of the instability region, producing ψ_0. This is because a systematic entropy flow is needed through the instability circle C from outside to inside of the instability region, so that the flow contributes additively to the internal entropy production there:

$$\frac{d}{dt}\int_I\left(-\log\frac{\psi}{\psi_0}\right)\psi da=\frac{dS_e}{dt}+\frac{dS_i}{dt}\,,$$
$$\frac{dS_e}{dt}\equiv\int_C\left(-\log\frac{\psi}{\psi_0}\right)\psi V dl>0\,,$$
$$\frac{dS_i}{dt}\equiv\int_I\left(\left(\frac{\partial}{\partial x}\log\frac{\psi}{\psi_0}\right)^2+\left(\frac{\partial}{\partial y}\log\frac{\psi}{\psi_0}\right)^2\right)\psi da>0\,. \tag{6·9}$$

The grow of the peak at around the minimum circle of ϕ is a consequence of the flow which results in

$$\frac{d}{dt}\int_o\left(-\log\frac{\psi}{\psi_0}\right)\psi da<0\,. \tag{6·10}$$

(I and O denote the inside and outside of the instability region.)
We examine these predictions by computing explicitly time-dependent solutions of the laser Fokker-Planck equation (6·1). Details will be reported in the near future. (See Note added in proof.)

Acknowledgement

The author wishes to express hearty thanks to Professor N. Hashitsume for providing an account of his old work and useful comments on the present manuscript.

References

1) A. Einstein, *Investigations on the Theory of the Brownian Motion*, edited by R. Fürth, translated by A. D. Cowper (Dover Pub. Inc., New York, 1956).
2) *Selected Papers on Noise and Stochastic Processes,* edited by N. Wax (Dover Pub. Inc., New York, 1954).
3) M. S. Green, J. Chem. Phys. **20** (1952), 1281.
4) N. Hashitsume, Prog. Theor. Phys. **8** (1952), 461.
5) P. Glansdorff and I. Prigogine, *Thermodynamic Theory of Structure, Stability and Fluctuations* (Wiley-Interscience, London, 1971).
6) For general backgrounds, see S. R. De Groot and P. Mazur, *Non-equilibrium Thermodynamics* (North Holland, Amsterdam, 1962).
7) P. Glansdorff and I. Prigogine, Physica **30** (1964), 351.
8) R. Graham, *Quantum Statistics in Optics and Solid-State Physics,* Springer Tracts in Modern Physics (Springer-Verlag) **66** (1973).
8′) R. Graham, *Fluctuations, Instabilities and Phase Transitions,* edited by T. Riste (Plenum Press, New York, London, 1975), p. 215.
9) J. L. Doob, *Stochastic Processes* (Wiley, New York, 1953).
10) N. G. Van Kampen, Physica **25** (1959), 1294.
11) H. Hasegawa, Prog. Theor. Phys. **55** (1976), 90.
12) R. Graham and H. Haken, Z. Phys. **245** (1971), 141.
13) H. Risken, *Statistical Properties of Laser Light,* Progress in Optics **8**, edited by E. Wolf (North-Holland, Amsterdam, 1970), p. 239.
14) R. Graham, *Proceedings of the International 3rd Rochester Conference on Coherence and Quantum Optics,* edited by Mandel and Wolf (Plenum Press, 1973), p. 851.
15) H. Hasegawa, Prog. Theor. Phys. **56** (1976), 44.
16) H. Hasegawa, Prog. Theor. Phys. **58** (1977) No. 1.

Note added in proof: The numerical analyses of the laser instability from the present standpoint by using the variational method[16] have been successfully carried out by S. Sawada, which will be presented at the 4th Rochester Conference on Coherence and Quantum Optics (1977).