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New Optimality Theory in Nature

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Various optimal shapes can be determined by making a certain objective function maximum or minimum and the optimal design in engineering is such a typical example. In the present paper, in the light of the concept of stability, a new general optimality theory for nonlinear nonequilibrium processes in nature will be proposed only through the first and second laws of thermodynamics and the existence of fluctuation in the natural world and then some important phenomenological observations in the field of life science will be explained as the examples of application of this new theory.

INTRODUCTION

The idea that nature pursues economy in all her working is one of the oldest principle of theoretical science from the time of Greeks to the present day(Rosen:1967). In other words, this idea is considered to mean that nature prefers optimality in all her economical working.

In thermodynamically equilibrium processes, we have already had Gibbs'general variational theory, which has greatly contributed to understanding the classical equilibrium phenomena of physics. On the other hand, in nonequilibrium processes, we have not yet had such a useful variational theory. This fact makes it difficult for us to understand the evolution of nonequilibrium phenomena in nature.

However, we have the following phenomenological observations for vital phenomena, which are typical examples in nonlinear nonequilibrium phenomena in natute. Roux asserted that all the living things produced their bodies from the minimum quantity of materials, operated their vital phenomena in the most effective way and hence were considered to be subjected to the minimum or maximum principles(Takeda:1983). Moreover, Lotka for the first time investigated the relationship between energy conversion and living things systematically and recognized the similar regularity to Roux's observation(Takeda:1983). Such a property in living things is called teleonomy(Monod:1971). The above observations imply that living things have the optimal functions and shapes for their activities in their environments and give us very deep overtone for the formulation of some general optimality theory by which the pattern formation and morphogenesis are analyzable.

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In addition, as is suggested by Gibbs' theory and the well known principle of minimun potential energy in the elasticity, etc., it is considered that the maximum or minimum property is often the counterpart of stability.

In the present paper, in the light of concept of stability, a new general optimality theory for nonlinear nonequilibrium processes in nature will be formulated only through the first and second laws of thermodynamics and the existence of fluctuation in the natural world and then some theoretically unresolved problems in the life science will be explained by application of this new theory.

BASIC CONCEPT FOR FORMULATION OF NEW THEORY

Here, based on the well known concept of stability, the nonequilibrium phenomenon is considered below.

First of all, let us begin with calling to our mind the definition of stability: if a nonequilibrium phenomenon to which any infinitesmal perturbation is applied and does not evolve into some other nonequilibrium phenomenon qualitatively different from the one before the application of infinitesmal perturbation, the nonequilibrium phenomenon is stable.

It is noticed that the founders of the thermodynamics in the 19th century had not yet recognized the existence of fluctuation in the natural world. However, since the Einstein theory of Brownian motion, the existence and importance of internal fluctuation which stems from the thermal molecular motions and external fluctuation from the outer world have gradually been recognized especially in nonlinear nonequilibrium phenomena. It is considered that the fluctuations play a role of the above mentioned perturbation in all nonequilibrium phenomena and so the nonequilibrium phenomena with no qualitative change for a finite length of time in spite of the existence of fluctuations, which we can often observe, should be stable by the above mentioned definition of stability. Thus, the definition of stability implys the existence of potential wall governing the returnability of fluctuating path as illustrated in Fig.1, which shows an example of a frequently fluctuating nonequilibrium phenomenon.

It is considered that the maximum or minimum property of physical phenomena results from the potential wall governing the returnability in the

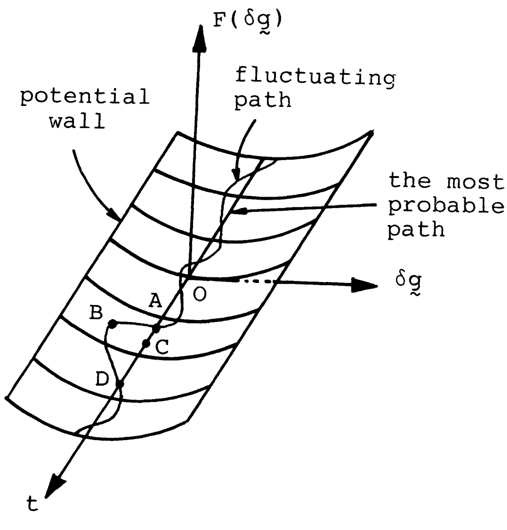

Fig. 1

definition of stability irrespective of the constitutive equations in each individual natural phenomenon and is the counterpart of stability.

In addition, all the related energy including the dissipative energy through fluctuations should be subject to the first law of thermodynamics and also we pay attention to the fact that if microscopic fluctuations are taken into consideration, the macroscopic physical laws become statistical like the Langevin equation derived from Newton' second law of motion.

NEW OPTIMALITY THEORY IN NATURE

Let us formulate a new general optimality theory for nonlinear nonequilibrium processes through the first and second laws of thermodynamics and the existence of fluctuation. For simplicity, let us use the Eulerian description referred to rectangular Cartesian co-ordinates $X_i (i=1,2,3)$ and consider a nonequilibrium thermodynamical system. The first law of thermodynamics in the local form is written as

$$\rho\dot{e} = \sigma_{ij}d_{ij} + q_{i,i} + \rho r \tag{2.1}$$

where $$d_{ij} = (v_{i,j} + v_{j,i})/2 \tag{2.2}$$

and ρ, $\dot{e}$, σ_{ij}, q_i, r and v_i are the density, the internal energy density per unit mass, the stress tensor, the heat flux vector, the heat radiation per unit mass and the velocity vector respectively and the superposed dot denotes the material derivative. The rate of total specific entropy $\dot{S}$ is composed of the rate of entropy production ${}_i\dot{S}$ which results from a nonequilibrium phenomenon in the system and the entropy flux ${}_e\dot{S}$ which flows into or out of the system:

$$\dot{S} = {}_i\dot{S} + {}_e\dot{S} \tag{2.3}$$

where ${}_e\dot{S}$ is defined in this case by

$$\rho\,{}_e\dot{S} = (q_i/\theta)_{,i} + \rho(r/\theta) \tag{2.4}$$

and θ is the absolute temperature. Then, the second law of thermodynamics is expressed as

$${}_i\dot{S} \geqq 0 \tag{2.5}$$

Referring to Eq.(2.4), paying attention to the relationship between the rate of entropy production ${}_i\dot{S}$ and the physical quantities in Eq.(2.1) such as dimension and combining Eq.(2.1) and (2.5), we have

$$\rho\theta\,{}_i\dot{S} \geqq \rho\dot{e} - (\sigma_{ij}d_{ij} + q_{i,i} + \rho r)\ (=0) \tag{2.6}$$

or $$\rho\theta\,{}_i\dot{S} \geqq \sigma_{ij}d_{ij} + q_{i,i} + \rho r - \rho\dot{e}\ (=0) \tag{2.7}$$

It is noticed that these inequalities essentially consist only of first and second laws of thermodynamics as is clear from the form of them.

Here, let us consider the consistency of the inequalities (2.6) and (2.7) with the above mentioned thermodynamics. From the inequality(2.7) and Eq.(2.4), we obtain

$$\rho({}_i\dot{S} - {}_e\dot{S} + \dot{e}/\theta) - \sigma_{ij}d_{ij}/\theta + q_i(\theta^{-1})_{,i} \geqq 0 \tag{2.8}$$

but, this inequality is contradictory to the following Clausius-

Duem inequality derived from Eqs.(2.1),(2.3),(2.4) and (2.5).

$$\rho({}_i\dot{S} + {}_e\dot{S} - \dot{e}/\theta) + \sigma_{ij}d_{ij}/\theta - q_i(\theta^{-1})_{,i} \geqq 0 \qquad (2.9)$$

On the other hand, the result obtained from Eq.(2.4) and the inequality(2.6) is consistent with the inequality(2.9). Thus, the combined form of Eqs.(2.1) and (2.5) is limited to the inequality (2.6). In the preceding consideration in this section, the microscopic fluctuation is not taken into account.

Next, let us consider the effect of the microscopic fluctuation in nonequilibrium phenomena below. As explained in the previous section, the founders of thermodynamics had not yet recognized the existence of fluctuation in nature but, at the present time, the existence and importance of fluctuation are sufficiently recognized. Thus, it is considered that all the conventional macroscopic physical laws such as the first and second laws of thermodynamics are statistical if the effect of microscopic fluctuation is taken into account but in stable states, usually, neglecting the meaningless microscopic fluctuation like a kind of noise, we just describe the physical laws by use of the most probable or average values to avoid unnecessary complexity.

However, as explained in the previous section, in nature the fluctuation plays a role of perturbation in the definition of stability and so the fluctuation is very important for the examination of stability in nonlinear nonequilibrium phenomena.

Here, let us introduce the microscopic fluctuation into the first law of thermodynamics(2.1) in the conventional macroscopic description and rewrite Eq.(2.1) for a fluctuating state as

$$F(\delta \underset{\sim}{g}) = \rho\dot{e} - (\sigma_{ij}d_{ij} + q_{i,i} + \rho r) \qquad (2.10)$$

where $\delta \underset{\sim}{g}$ denotes some perturbation from the path with no fluctuation which is included in various physical quantities in the right hand of Eq.(2.10) and $F(\delta \underset{\sim}{g})$ defined by Eq.(2.10) is called the fluctuation function. It is noticed that Eq.(2.10) is the description for the first law of thermodynamics in a fluctuating state and along the most probable or average path ACD with no fluctuation in Fig. 1, by virtue of the first law of thermodynamics(2.1) in the conventional macroscopic description, we should have

$$F(\underset{\sim}{0}) = \rho\dot{e} - (\sigma_{ij}d_{ij} + q_{i,i} + \rho r) = 0 \qquad (2.11)$$

In the following, let us consider the property of $F(\delta \underset{\sim}{g})$ in a fluctuating state. As explained in the previous section, in spite of the existence of fluctuation the nonequilibrium phenomenon is frequently stable in nature, from the definition of stability this fact means the dissipation of fluctuating energy and further,from the viewpoint of statistical mechanics, the dissipation of energy is considered to result from the randomization of regular direction of a energy flow through the fluctuation. In addition, though there always exist fluctuations, the nonequilibrium phenomenon with negative rate of entropy production has never observed since the establishment of the second law of thermodynamics. Thus, the second law of thermodynamics(2.5) is still valid for a fluctuating state. It is noticed that the relationship between the right hand side and the left one of the inequality(2.6) essentially depends only on the second law of thermodynamics (2.5) and so the inequality(2.6) is considered to be applicable to a fluctuating state. Combining the inequality (2.6) and Eq.(2.10), we have

$$\rho\theta\,{}_i\dot{S} \geqq \rho\dot{e} - (\sigma_{ij}d_{ij} + q_{i,i} + \rho r) = F(\delta \underset{\sim}{g}) \qquad (2.12)$$

Requiring that even if any internal or external perturbation such as a fluctuation acts upon a nonequilibrium phenomenon, the rate of entropy production should always be positive, the following thermodynamical variational inequality is obtained.

$$\rho\dot{e} - (\sigma_{ij}d_{ij} + q_{i,i} + \rho r) = F(\delta \underset{\sim}{g}) > 0 \tag{2.13}$$

It is noticed that we have selected the case of positive rate of entropy production from two possibility in Eq.(2.5), i.e. positive rate or zero and as long as the above inequality holds, the possibility that the rate of entropy production becomes negative or zero is completely denied through the inequality(2.13),i.e. the rate of entropy production is always positive. This fact means that the available energy and fluctuating one in the nonequilibrium phenomenon are always dissipated and therefore this phenomenon is stable.

Furthermore, considering the first law of thermodynamics (2.10) in the microscopic description along a fluctuating path ABD in Fig. 1 under the condition(2.13), we have

$$\Delta F_{AB} + \Delta F_{BD} = 0 \tag{2.14}$$

This fact is closely related to the translational symmetry and means that Eqs.(2.10) and (2.13) are consistent with the first law of thermodynamics(2.1) in the conventional macroscopic description. Combining Eq.(2.11) and the inequality (2.13), we get

$$\rho\dot{e} \geqq \sigma_{ij}d_{ij} + q_{i,i} + \rho r \tag{2.15}$$

In the following, we consider the case that the rate of entropy production is always zero:

$${}_i\dot{S} = 0 \tag{2.16}$$

In this case, Eq.(2.12) reduces to

$$\rho\theta_i\dot{S} = \rho\dot{e} - (\sigma_{ij}d_{ij} + q_{i,i} + \rho r) = F(\delta \underset{\sim}{g}) \tag{2.17}$$

Requiring that the rate of entropy production is zero for any internal or external perturbation such as a fluctuation, we have

$$\rho\dot{e} - (\sigma_{ij}d_{ij} + q_{i,i} + \rho r) = F(\delta \underset{\sim}{g}) = 0 \tag{2.18}$$

This equation expresses that the potential wall for fluctuation is flat, means that a fluctuation which has once arised continues to exist without growth or decay and corresponds to the marginal state of stability.

Finally, let us consider the case that the rate of entropy production is always negative in a fluctuating state. However, the nonequilibrium phenomenon satisfying this condition has never been observed historically though there always are fluctuations and so such a phenomenon is considered to be unstable and unrealizable in nature. So, we discuss nothing further for this case.

Now, let us turn our attention to the formulation of global form. Denoting the body force vector and the surface traction vector by $\hat{f}_i$ and $\hat{t}_i$ respectively, the equation of conservation of mass and the equations of balance of momenta are written as

$$\dot{\rho} + \rho v_{i,i} = 0 \tag{2.19}$$

$$\sigma_{ij,j} + \hat{f}_i = \rho\dot{v}_i \tag{2.20}$$

and the boundary conditions:

$$\sigma_{ij}n_j = \hat{t}_i \qquad \text{on } \partial V_\sigma \tag{2.21}$$

$$v_i = \hat{v}_i \quad \text{on } \partial V_v \tag{2.22}$$

are also specified. Integrating the inequality(2.6) over the volume V of the system, using the Gauss-Green theorem, the equations of balance of momenta(2.20), the relation between deformation rate tensor and velocity vector(2.2) and the boundary conditions (2.21) and (2.22) and then giving the similar consideration to the case of Eq.(2.15), we obtain

$$\dot{K} + \dot{E} \geqq W + Q \tag{2.23}$$

where

$$\dot{K} = \int_V \rho v_i \dot{v}_i dv \tag{2.24}$$

$$\dot{E} = \int_V \rho \dot{e} dv \tag{2.25}$$

$$W = \int_V \hat{f}_i v_i dv + \int_{\partial V_\sigma} \hat{t}_i v_i ds + \int_{\partial V_v} t_i \hat{v}_i ds \tag{2.26}$$

$$Q = \int_{\partial V} q_i n_i ds + \int_V \rho r dv \tag{2.27}$$

It is notice that the signs of inequality and equality in Eq. (2.23) hold for any fluctuating state and the most probale or average one respectively. We call the right and left hand sides of Eq.(2.23) active and passive powers respectively. Let us consider Eq.(2.23) in more detail. If the left and right hand sides of this equation take the most probable value and a fluctuating value respectively, we have

$$[\ \dot{K} + \dot{E}\ ]^* \geqq W + Q \tag{2.28}$$

where [K + E]* expresses the most probable value of [K + E]. Eq.(2.28) is rewritten into the following equivalent form:

$$[\ \dot{K} + \dot{E}\ ]^* = [\ w + Q\ ]_{max.} \tag{2.29}$$

On the other hand, if the right and left hand sides of Eq.(2.23) have the most probable value and a fluctuating one respectively, we get

$$\dot{K} + \dot{E} \geqq [\ W + Q]^* \tag{2.30}$$

where [W + Q]* expresses the most probable value of [W + Q]. Eq.(2.30) is rewritten into the following equivalent form:

$$[\ \dot{K} + \dot{E}\ ]_{min.} = [\ W + Q\ ]^* \tag{2.31}$$

By the first law of thermodynamics in the conventional macroscopic description, the most probale values of the left and right hand sides of the inequality(2.23) should be equal:

$$[\ \dot{K} + \dot{E}\ ]^* = [\ W + Q\ ]^* \tag{2.32}$$

Therefore, from Eqs.(2.29),(2.31) and (2.32), we have

$$[\ \dot{K} + \dot{E}\ ]_{min.} = [\ W + Q\ ]_{max.} \tag{2.33}$$

This equation means that the active power and the possive one compete each other through fluctuations and as the result of it a cooperative or harmonic state in the macroscopic sense is formed.

In addition, it is noticed that as is clear from Eq.(2.18), we cannot expect the maximum or minimum property for the macroscopic solution of physical phenomena in the marginal stability.

APPLICATIONS OF NEW THEORY TO LIFE SCIENCE

First of all, we should pay attention to the fact that all the stable nonequilibrium phenomena are subjected to the first and second laws of thermodynamics, the fluctuation always exists in nature and therefore the results obtained from the present theory which is derived through these two laws and the effect of fluctuation ought to be common in all stable nonequilibrium phenomena.

Now, let us consider many biologists' belief(Katchalsky & Curran:1965) that the evolution of living things dissipates the least energy. This belief is eqivalent to the fact that living things operate in the maximum efficiency and is deeply concerned with Roux and Rotka'observation. The Helmholtz free energy per unit mass is defined by

$$\phi = e - \theta S \tag{3.1}$$

Substituting this equation and Eq.(2.3) into Eq.(2.6) and then giving the similar consideration to the case deriving Eq.(2.33) from Eq.(2.6), we have

$$\begin{aligned}[-\dot{K} - \int_V \rho(\dot{\phi} + \theta\dot{S} + \theta_e\dot{S})dv + \int_V \hat{f}_i v_i dv + \int_{\partial v_\sigma} \hat{t}_i v_i ds \\ + \int_{\partial v_v} t_i \hat{v}_i dv + \int_{\partial v} q_i n_i ds + \int_V \rho r dv\,]_{max.} = [\int_V \rho\theta_i \dot{S}\,]_{min.}\end{aligned} \tag{3.2}$$

This equation expresses that a natural phenomenon evolves towards the direction in which the dissipative energy is minimum and is consistent with the above mentioned many biologists'belief.

Denoting the rates of total input and output energy including the heat energy by W_i and W_o , rewriting Eq.(2.23) by use of them

$$(\dot{K} + \dot{E})/W_i \geqq (W_i - W_o)/w_i \tag{3.3}$$

and then giving the similar consideration to the case deriving Eq. (2.33) from Eq.(2.23), we obtain

$$[(\dot{K} + \dot{E})/W_i]_{min.} = [(W_i - W_o)/W_i]_{max.} \tag{3.4}$$

where, it is noticed that W_i and W_o are positive. $(W_i - W_o)/W_i$ is the definition of efficiency itself and the right hand side of the above equation expresses that a nonequilibrium phenomenon spontaneously operates in the maximum efficiency. In addition, recently the above mentioned many biologists'belief has strongly been supported through numerical simulations by Nishiyama and Shimizu(1981).

Next, let us consider Lotka's phenomenological opinion based on his ecological observation in nature(Lotka:1945,1957) by application of the present theory. Thruogh his deep systematic observation in nature, Lotka recognized that there were two opposing tendencies in nature i.e. a promotion and a retardation of dissipative process which were going on side by side. In other words, the former is the tendency that the cosmic effect of the scrimmage for available energy increases the total energy flux or the rate of degradation of the energy received from the sun and the latter is the tendency that greater efficiency in utilizing energy, a better husbanding of resources and hence a less rapid drain must work to the advantage of a species talented in that direction. Lotka also explained that natural selection tended to make the flux through the system a maximum, so far as compatible with the constraints to which the system is subject. It is considered that the maximization of energy flux through the system and the constraints to which the system is subjected correspond to the former and latter tendencies respectively in the above explanation.

In the following, let us consider the relation between Lotka's opinion and our optimality theory. Rewriting Eq.(2.33) by use of W_i and W_o , we have

$$[\dot{K} + \dot{E}]_{min.} = [W_i - W_o]_{max.} \tag{3.5}$$

The right hand side of Eq.(3.5) explains the former tendency that the energy flux through the system or the rate of degradation of the energy received from the sun is maximum of the permissible energy flux. On the other hand, the left hand side of Eq.(3.5) expresses that the rate of change of the sum of kinetic energy and internal energy consisting of the Helmholtz free energy, the entropy production, etc. of the system concerned is minimum of the permissible rate and this minimum rate of change retards the energy flux through the system. This fact corresponds to the latter tendency in Lotka's opinion. Thus, it is considered that Eq.(3.5) well explains two opposing tendencies in nature which were stated by Lotka.

CONCLUDING REMARKS

A general theoretical foundation has been given for the idea that nature pursues the optimality in all her economical working. As is clear from the formulation procedure, the range of applicability of the present theory is equivalent to that of the first and second laws of thermodynamics except the case that the rate of entropy production is zero and therefore, this theory is considered to explain the greatest common property in stable natural phenomena. In addition, this optimality theory has already been applied to various kinds of problems (Niiseki:1981,1982,1986) besides those of the life science explained here.

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