Theory of Non-equilibrium Thermodynamics in the Optimal Control Processes Part I: Mathematical Formulation

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The theory of non-equilibrium thermodynamics in the optimal control processes is established, by using the Pontryagin's theory of optimal control and the Bellman's theory of dynamic programming, for the first time. For this theory, we study the systems of nonlinear differential equations $\dot{\vec{x}} = \vec{f}(\vec{x}, \vec{u}, t)$ of the state variables $\vec{x}$ under the condition that the control variables $\vec{u}$ be optimal. It is the natural generalization of Onsager-Prigogine's theory of the irreversible processes to the theory of the optimal control processes. It is shown that the principle of the least dissipation of energy by Onsager and the principle of the least production of entropy should be generalized to the principle of the optimal dissipation of energy and the principle of the optimal production of entropy, respectively. In this theory, it is shown that for the system of the optimal control processes, the Pontryagin's Hamiltonian plays the same role of the Hamiltonian in classical mechanics, while the Bellman's optimality equation plays the same role of the Hamilton-Jacobi equation, respectively. The main result is summarized as follows: Define the Pontryagin's Hamiltonian $\mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t)) \equiv \vec{\psi}(t) \cdot \vec{f}(\vec{x}, \vec{u}, t) + T[\dot{S}(\vec{x}, \vec{u}) - \Phi(\vec{x}, \vec{u})]$, where $\dot{S}(\vec{x}, \vec{u})$ means the entropy production and $\Phi(\vec{x}, \vec{u})$ the dissipation function of energy, respectively. Then, the following Pontryagin's Hamilton dynamics must be satisfied:

$$\frac{d\vec{x}(t)}{dt} = \frac{\partial \mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t))}{\partial \vec{\psi}}, \quad \frac{d\vec{\psi}(t)}{dt} = -\frac{\partial \mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t))}{\partial \vec{x}},$$

with the optimality condition:

$$\frac{\partial \mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t))}{\partial \vec{u}} = \vec{\psi}(t) \cdot \frac{\partial \vec{f}(\vec{x}, \vec{u})}{\partial \vec{u}} + T\left[\frac{\partial \dot{S}(\vec{x}, \vec{u})}{\partial \vec{u}} - \frac{\partial \Phi(\vec{x}, \vec{u})}{\partial \vec{u}}\right] = 0.$$

It is the generalization of the Onsager-Prigogine's theory with the extremum condition $\delta\left[\dot{S}(\alpha, \dot{\alpha}) - \Phi(\dot{\alpha}, \dot{\alpha})\right] = 0$ for the deviation α of the state variable from its equilibrium value to that for the optimal control systems. The proofs and the details will be presented in this paper.

I. INTORDUCTION

A. Preliminary Motivation

One of the main goals of theoretical physics is to understand the nature of non-equilibrium states such as life and living things in nature. These systems are frequently called the systems *far-from equilibrium*. Living organisms are made by a collection of various materials that are in non-equilbrium states. Materials are in equilibrium states as usual matters, once they exist separately as independent materials. However, once they belong to a living organism as its parts, they become able to play an important role as key ingredients in the life system. This reason is not yet known as a long standing problem.

In order to answer this kind of problem, it seems to us that we have to find a new principle going beyond so-called the *two laws of thermodynamics* – (i) the first law: *the energy conservation law*; (ii) the second law: *the entropy increasing law*. These were constructed for the system of isolated physical systems.

B. Carnot's Principle in Classical Thermodynamics

There is a long history for thermodynamics[1–4]. First, Carnot formulated the Carnot engine in order to eluciadte the concept of entropy: the entropy S is defined by

$$dS = \frac{d'Q}{T}, \tag{1}$$

or equivalently,

$$S(\alpha) = \int_{\alpha_0}^{\alpha} \frac{d'Q}{T}, \tag{2}$$

where Q is the heat supplied to the system and T the temperature of the system. The transition from the initial thermal equilibrium state α_0 to the final thermal equilibrium state α is quasistatic. And d' usually means that the transition process depends upon the path of the process.

The concept of the energy conservation law is given by

$$dE = d'Q - P^{(e)}dV + \sum_i F_i^{(e)} dx_i + \sum_{j=1}^{c} \mu_j^{(e)} dN_j, \tag{3}$$

where E is the internal energy of the system, $P^{(e)}$ the external pressure, V the volume of the system, $F_i^{(e)}$ the the i-th

force from the external, x_i the coordinate of the system, N_j the molecular number of the j-th species in the system, and $\mu_j^{(e)}$ the chemical potential of the j-th species, respectively. c is the number of species in the system.

In this case of thermodynamics for the equilibrium state, the system is thermally equilibrium to the external environment. Hence, all external variables can be replaced by the variables for the system:

$$dE = TdS - PdV + \sum_i F_i dx_i + \sum_j \mu_j dN_j, \tag{4}$$

where P is the internal pressure, V the volume of the system, F_i the the i-th force from the external, x_i the coordinate of the system, N_j the molecular number of the j-th species in the system, and μ_j the chemical potential of the j-th species, respectively. From the two laws of thermodynamics, we find the general condition for equilibrium:

$$\delta E - T^{(e)}\delta S + P^{(e)}\delta V - \sum_i F_i^{(e)}\delta x_i - \sum_j \mu_j^{(e)}\delta N_j \geq 0. \tag{5}$$

C. Gibbs-Duhem's Principle in Equilibrium Thermodynamics

Using the energy conservation law together with the second law of thermodynamics, Mayer, Joule, Thomson and Clausius established so-called the *classical thermodynamics*. From this, the so-called Gibbs-Duhem's relation[5]:

$$SdT - VdP + \sum_j N_j d\mu_j = 0. \tag{6}$$

is obtained. And all thermodynamic inequalities are derived[2] as follows: Let denote the internal energy E by the potential U. Let us denote the thermodynamic *intensive* variables $T, -p, F_1, F_2, \cdots, \mu_1, \mu_2, \cdots$ by $y_1, y_2, \cdots$. And denote the thermodynamic *extensive* variables $S, V, x_1, x_2, \cdots, N_1, N_2, \cdots$ by $Y_1, Y_2, \cdots$, where

$$y_i = \frac{\partial U}{\partial Y_i}. \tag{7}$$

The second variation of the potential is given by

$$\delta^2 U = \frac{1}{2}\sum_i \sum_k \frac{\partial^2 U}{\partial Y_i \partial Y_k}\delta Y_i \delta Y_k = \frac{1}{2}\sum_i \delta Y_i \delta y_i. \tag{8}$$

Therefore, the thermal equilibrium condition is

$$\delta^2 U = \frac{1}{2}\sum_i \sum_k \frac{\partial^2 U}{\partial Y_i \partial Y_k}\delta Y_i \delta Y_k = \frac{1}{2}\sum_i \delta Y_i \delta y_i \geq 0, \tag{9}$$

or,

$$\sum_i \delta Y_i \delta y_i \equiv \delta T \delta S - \delta p \delta V + \sum_i \delta F_i \delta x_i + \sum_j \delta \mu_j \delta N_j \geq 0. \tag{10}$$

Then, the condition that the second variation is positive is given as

$$\begin{vmatrix} \frac{\partial^2 U}{\partial Y_{k_1}^2} & \frac{\partial^2 U}{\partial Y_{k_1}\partial Y_{k_2}} & \cdots & \frac{\partial^2 U}{\partial Y_{k_1}\partial Y_{k_n}} \\ \frac{\partial^2 U}{\partial Y_{k_2}\partial Y_{k_1}} & \frac{\partial^2 U}{\partial Y_{k_2}^2} & \cdots & \frac{\partial^2 U}{\partial Y_{k_2}\partial Y_{k_n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 U}{\partial Y_{k_n}\partial Y_{k_1}} & \frac{\partial^2 U}{\partial Y_{k_n}\partial Y_{k_2}} & \cdots & \frac{\partial^2 U}{\partial Y_{k_n}^2} \end{vmatrix} \geq 0. \tag{11}$$

where, $n = 1, 2, \cdots$, and $Y_{k_1}, \cdots, Y_{k_n}$ are arbitrary n individuals out of $Y_1, Y_2, \cdots$. From this condition, the *principle of Le Chatelier-Braun* is proved[2–4].

D. Boltzmann's Principle in Statistical Mechanics

And later, Maxwell, Boltzmann and Gibbs succeeded to found the *statistical mechanics* for the basis of thermodynamics of equilibrium states[6], using the *Boltzmann's principle*:

$$S = k_B \log W, \tag{12}$$

where k_B is the Boltzmann constant and W the total number of the partition of the states. Although the statistical mechanics of Gibbs has been successfully applied to many areas of physics, such are almost all equilibrium systems. Otherwise, it is not successful to do so.

E. Need for the Non-equilibrium Thermodynamics

This problem traces back to the origin or birth of the thermodynamics in which formalism there is no time difference dt, since the difference d or d' in thermodynamics means the one between the physical quantities in different states in equilibrium. For example, dE means the difference of the internal energy E of the system between two independent equilibrium states. Therefore, there is no room for time to enter the problem explicitly. In other words, in the standard thermodynamics theory we ignore the time-development of the system apparently. Otherwise, we cannot calculate thermodynamic quantities. This is good for the equilibrium systems such as solids or dead objects, but not so good for the non-equilibrium systems as well as the systems far-from equilibrium such as life or living objects. Thus, we need find another way of thinking such non-equilibrium and/or systems far-from equilibrium so that one can establish the absolute theory of the non-equilibrium thermodynamics.

To go in this direction, we need find as a generalization of Eq.(4) something like

$$\mathcal{W} \equiv \frac{dE}{dt} = T\frac{dS}{dt} - P\frac{dV}{dt} + \sum_i F_i \frac{dx_i}{dt} + \sum_j \mu_j \frac{dN_j}{dt}. \tag{13}$$

If this is true, then this relation states that the internal energy creation in time is balanced between the entropy creation in time, the energy supply in time and the energy consumption in time, etc. The internal energy creation is nothing but the

work rate $\mathcal{W}$ of the system; this quantity is measured in a unit of Watts [= Joules/sec]. And if this kind of the relation holds true, then one can calculate the instantaneous energy change of the system systematically. Hence, there appears a possibility to consider the systems far-from equilibrium. It will be very nice. The main goal of the present paper is to establish this kind of theory.

II. FORMALISM OF CLASSICAL MECHANICS

Before going to do so, let us first reimind us of the formalism of classical mechanics[7] for a moment for the later purposes.

A. Hamilton's Principle in Classical Mechanics

The *Hamilton's principle* in classical mechanics is the principle for classical variables. Suppose that there is a Hamiltonian H that is given by classical variables of coordinates $\vec{x}$ and momenta $\vec{p}$ such that $H = H(\vec{x}, \vec{p})$. Now we have the following Hamilton equations:

$$\frac{d\vec{x}}{dt} = \frac{\partial H}{\partial \vec{p}}, \quad \frac{d\vec{p}}{dt} = -\frac{\partial H}{\partial \vec{x}}. \tag{14}$$

This provides the Newton equation for a particle of mass m under a potential $V(\vec{x})$ if we apply $H = \frac{\vec{p}^2}{2m} + V(\vec{x})$ for the Hamiltonian such that

$$\frac{d\vec{x}}{dt} = \frac{\vec{p}}{m} = \vec{v}, \quad \frac{d\vec{p}}{dt} = -\frac{\partial V(\vec{x})}{\partial \vec{x}}. \tag{15}$$

Obviously, the Hamiltonian is time-independent, which means that the Hamiltonian is a conserved quantity under the development of time. This can be proven quickly such as

$$\frac{dH}{dt} = \frac{\partial H}{\partial \vec{x}} \cdot \frac{d\vec{x}}{dt} + \frac{\partial H}{\partial \vec{p}} \cdot \frac{d\vec{p}}{dt} = \frac{\partial H}{\partial \vec{x}} \cdot \frac{\partial H}{\partial \vec{p}} - \frac{\partial H}{\partial \vec{p}} \cdot \frac{\partial H}{\partial \vec{x}} = 0, \tag{16}$$

where we have used Eq.(14) in the last step.

B. Least Action Principle in Classical Mechanics

On the other hand, there is the *least action principle* in classical mechanics. Suppose that the action S is represented by the Lagrangian $L = L(\vec{x}, \dot{\vec{x}})$ such that

$$S = \int_{t_0}^{t_1} L\, dt = \int_{t_0}^{t_1} L(\vec{x}, \dot{\vec{x}})\, dt. \tag{17}$$

If the action S is *minimal*, then the variation δS must satisfy

$$\delta S = 0. \tag{18}$$

From this extremum condition, we obtain the so-called Euler-Lagrange equation:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\vec{x}}}\right) - \frac{\partial L}{\partial \vec{x}} = 0. \tag{19}$$

This means that as long as the orbit follows the Euler-Lagrange equation, the value of the action can be minimized. In this sense the meaning of the action for classical mechanics is a kind of evaluate function so that we can find an optimal orbit under the physical condition.

Although the least action principle is so powerful enough to apply to many problems of classical mechanics, this concept stands up on the *two-boundary-value problem*. This comes from the history that the variational problem was developed from solving the two-boundary-value problems such as the brachistochrone curve or the catenary problem. Therefore, even for determining the dynamical orbit of a body in the course of time, we have to put both the initial and final condition before the orbit is found. This seems funny, because we do not yet know the final goal before we perform the phenomenon. Nevertheless, we have no other method to do so. In stead of meeting this difficulty we adopt the so-called *Hamilton-Jacobi method*.

C. Hamilton-Jacobi Equation in Classical Mechanics

When we regard one of the two times t_0 and t_1 as a free variable, then the action becomes a function of time. For example, suppose that the final time t_1 is a free parameter t. We now have

$$S(t) = \int_{t_0}^{t} L\, dt = \int_{t_0}^{t} L(\vec{x}, \dot{\vec{x}})\, dt. \tag{20}$$

This means that fixing the initial time t_0, we can change the final time t freely. However, in the course of time the orbit must follow the Equler-Lagrange equation of Eq.(19). Taking the time variation δS, we find

$$\delta S = \left[\frac{\partial L}{\partial \dot{\vec{x}}} \cdot \delta\vec{x}\right]_{t_1}^{t} + \int_{t_1}^{t} \left(\frac{\partial L}{\partial \vec{x}} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\vec{x}}}\right) \cdot \delta\vec{x} dt. \tag{21}$$

Since at the initial time t_0 we hold $\delta\vec{x}(t_0) = 0$ and the last term vanishes, the above equation becomes

$$\delta S = \frac{\partial L}{\partial \dot{\vec{x}}} \cdot \delta\vec{x}(t) = \vec{p} \cdot \delta\vec{x}(t), \tag{22}$$

where we have defined as

$$\vec{p} = \frac{\partial L}{\partial \dot{\vec{x}}}. \tag{23}$$

Now, if we differentiate S with respect to time t, then we obtain

$$\frac{dS}{dt} = L. \tag{24}$$

The left hand side of Eq.(24) is the total derivative of time. Therefore, if we use the partial derivative of time, then we have

$$\frac{dS}{dt} = \frac{\partial S}{\partial t} + \frac{\partial S}{\partial \vec{x}} \cdot \dot{\vec{x}} = \frac{\partial S}{\partial t} + \vec{p} \cdot \dot{\vec{x}} = L. \tag{25}$$

Let us define the Hamiltonian H as

$$H = \vec{p} \cdot \dot{\vec{x}} - L. \tag{26}$$

From Eq.(25) together with Eq.(26) provides

$$\frac{\partial S}{\partial t} + H = 0. \tag{27}$$

By Eq.(25) the momentum vector $\vec{p}$ is given by

$$\vec{p} \equiv \frac{\partial S}{\partial \vec{x}}. \tag{28}$$

Here, this means that the momentum is given by the gradient of the action. Therefore, finally we obtain the *Hamilton-Jacobi equation* as

$$\frac{\partial S(\vec{x}, t)}{\partial t} + H\left(\vec{x}, \frac{\partial S}{\partial \vec{x}}\right) = 0. \tag{29}$$

As described before, the Hamilton-Jacobi equation gives the time-development of the action along the course of the orbit, starting from the initial point. Therefore, in this approach we need not know the final time and position before the orbit reaches the final point. Instead, this needs at any instant that the orbit has to find the most optimal direction so that the least action is realized; this is realized that the momentum $\vec{p}$ is defined by the gradient of the action S.

D. Attractiveness of the Formulation of Classical Mechanics

What is most attractive in the formulation of classical mechanics is the following: Since the energy is conserved in a mechanical problem, it can be solved once the initial energy is given in the problem. And the mechanical system such as a pendulum or a spring moves automatically as if the energy is always conserved. So, as long as there is no dissipation of energy, once the initial energy is given to the system, then the system moves automatically and forever. This is our understanding on the physics of macroscopic mechanical objects.

As is described above, in classical mechanics all variables in the system are mechanical variables such as the coordinate vectors $\vec{x}$ and its momentum vectors $\vec{p}$. The set of the vectors $(\vec{x}, \vec{p})$ forms the so-called *phase space* for the Hamilton dynamics which is given by the Hamilton equations of motion.

On the other hand, in our problem of life or living things here, the system is described by the dynamical change of densities of molecules under chemical reactions. At a given time, the system is determined by the instantaneous values of densities in the system. Hence, we need treat the new type of variables – the *state variables* such as densities that are given as a sum of the sets of classical particles or objects. Therefore, we have to treat macroscopic state variables as mechanical variables of the system. This means that we regard a biologically living macroscopic system as a classical mechanical system given by regarding state variables as mechanical variables.

This point of view is interesting. In this view, as a pendulum moves automatically following the energy conservation law, the macroscopic biological system should be able to move automatically following some unknown law of physics, if such new type of law exists. This is our goal here. We would like to find such new principle of conservation law.

III. MODERN CONTROL THEORY AND PONTRYAGIN'S MAXIMUM PRINCIPLE

In this section, we are going to consider the essential concepts and the formalism of the so-called *Pontryagin's theory of optimal control*[8, 9] for the later purposes. This theory is the totally new type of extensions of the standard control theory[10] which is based upon the negative feedback mechanisms before 1960. Since then, the Pontryagin's theory was called the *modern control theory*, while the old control theory was called the *classical control theory*. This reminds us of what happened in the discovery of quantum mechanics.

On the other hand, theoretically speaking, the Pontryagin's theory of optimal control is the natural extension of the formalisms of Hamilton's principle and the least action principle in classical mechanics[7]. It was totally a revolution in theoretical physics as well. However, much has long been not so well-konwn in physics society. It seems because the revolution has occurred in the optimal control theory and the automatic control theory in engineering community around the year of 1960 and because the value of scientists of USSR was intentionally and absolutely ignored by western scientists at that time in the era of the cold war between USSR and USA.

A. Dynamical Equations of the System

In our problem here we have to consider typically the following equations[8, 9]:

$$\frac{d\vec{x}}{dt} = \dot{\vec{x}} = \vec{f}(\vec{x}, \vec{\lambda}, t), \tag{30}$$

namely,

$$\begin{cases} \dot{x}_1 &= f_1(x_1, \cdots, x_n, \lambda_1, \cdots, \lambda_m, t) \\ \dot{x}_2 &= f_2(x_1, \cdots, x_n, \lambda_1, \cdots, \lambda_m, t) \\ \vdots & \qquad\qquad \vdots \\ \dot{x}_n &= f_n(x_1, \cdots, x_n, \lambda_1, \cdots, \lambda_m, t) \end{cases}. \tag{31}$$

Here, $\vec{x}$ is the state vector and $\vec{\lambda}$ the external parameters.

This type of the equations is quite common in chaos theory and the so-called the theory of nonlinear phenomena. In these theories, we regard $\vec{\lambda}$ as constant vectors that are given initially. But, in the optimal control theory of Pontryagin, we regard $\vec{\lambda}$ as the *control variables* in the system. This is a philosophical jump between the theories, and it gives rise to a new level of physical theory. In order to distinguish between the external variables and the control variables, let us use $\vec{u}$ for the control variables instead of $\vec{\lambda}$. Hence, we have the following:

$$\frac{d\vec{x}}{dt} = \dot{\vec{x}} = \vec{f}(\vec{x}, \vec{u}, t), \tag{32}$$

namely,

$$\begin{cases} \dot{x}_1 &= f_1(x_1, \cdots, x_n, u_1, \cdots, u_m, t) \\ \dot{x}_2 &= f_2(x_1, \cdots, x_n, u_1, \cdots, u_m, t) \\ \vdots & \qquad\qquad \vdots \\ \dot{x}_n &= f_n(x_1, \cdots, x_n, u_1, \cdots, u_m, t) \end{cases}. \tag{33}$$

B. Pontryagin's Hamiltonian – the New Conservation Law

As in the case of classical mechanics, once we regard the state variables $\vec{x}$ as the classical variables, we can define a Hamiltonian. Let us define the Hamiltonian:

$$\mathcal{H} = \vec{\psi} \cdot \dot{\vec{x}} = \vec{\psi} \cdot \vec{f}(\vec{x}, \vec{u}, t), \tag{34}$$

where $\vec{\psi} = (\psi_1, \cdots, \psi_n)$ is an adjoint vector. According to the Pontryagin's theory of the optimal control[8, 9], we can prove the Hamilton equation:

$$\frac{d\vec{x}}{dt} = \frac{\partial \mathcal{H}}{\partial \vec{\psi}}, \tag{35}$$

$$\frac{d\vec{\psi}}{dt} = -\frac{\partial \mathcal{H}}{\partial \vec{x}}. \tag{36}$$

In order to escape from the confusion between the standard *Hamiltonian* in classical mechanics due to Hamilton and the Pontryagin's Hamiltonian in the optimal control theory, we would like to use the *Pontryaginian* or *Pontryagin's Hamiltonian* for the latter. This is because they are totally different from each other in a physical unit. Hamiltonian is given in a unit of *energy* [Joules], while Pontryaginian is given in a unit of *work rate,* $\frac{dE}{dt}$, or *power*, $\mathcal{W}$, [Joules/sec = Watts].

Eq.(35) provides nothing but the original equations of Eq.(32) by definition. Eq.(36) is something else. But it can be regarded as a generalization of the Gibbs free energy in Eq.(4).

To understand this point, let us suppose that $\vec{f}(\vec{x}, \vec{u}, t)$ does not depend upon $\vec{x}$ such as $\vec{f}(\vec{x}, \vec{u}, t) = \vec{f}(\vec{u}, t)$. In this case, Eq.(36) provides

$$\frac{d\vec{\psi}}{dt} = 0, \ \vec{\psi} = \text{const.} \equiv \vec{\mu}. \tag{37}$$

Substituting the above the original Pontryaginian of $\mathcal{H}$, we obtain

$$\mathcal{H} = \vec{\mu} \cdot \dot{\vec{x}} = \vec{\mu} \cdot \vec{f}(\vec{u}, t). \tag{38}$$

This is nothing but the standard time-derivative of Gibbs free energy: Since $G = \sum_j \mu_j N_j$, if we rewrite the set $(N_1, \cdots, N_n)$ as $\vec{x} \equiv (N_1, \cdots, N_n)$ and $\vec{\mu} \equiv (\mu_1, \cdots, \mu_n)$, we obtain

$$\frac{dG}{dt} = \sum_j \mu_j \frac{dN_j}{dt} = \vec{\mu} \cdot \dot{\vec{x}} = \mathcal{H}. \tag{39}$$

This expression means that the rate of Gibbs free energy is conserved under the time-development of the system. This is an indication of the existence of the dynamical relation like Eq.(13).

C. Proof of the New Conservation Law

The general proof of the conservation of the Pontryagin's Hamiltonian is quite complex. It is not so convenient to describe the detail in short here. Since the proof is given in the text book of Pontryagin et. al.[8, 9], we skip the detail. Therefore, we would like to describe the essence of the proof.

As before, we start with the dynamics given by Eq.(32) [or Eq.(33)]. Let us find the equilibrium state taking the variation $\delta\vec{x}$ such as

$$\vec{y}(t) = \vec{x}(t) + \varepsilon \delta\vec{x}(t), \tag{40}$$

where ε is a small positive value and we assume that the initial condition for $\delta\vec{x}$ such that it starts with the value:

$$\delta\vec{x}(t_0) = \vec{\xi}_0. \tag{41}$$

Substituting the above into Eq.(32), we can expand the original dynamical equations with respect to ε. Then, we can obtain the linearlized equations of motion:

$$\frac{d(\delta x_i)}{dt} = \sum_{j=1}^{n} \frac{\partial f_i(\vec{x}(t), \vec{u}(t))}{\partial x_j} \delta x_j \equiv \sum_{j=1}^{n} \Lambda_{ij} \delta x_j. \tag{42}$$

or in the vector notation we have

$$\frac{d(\delta\vec{x})}{dt} = \frac{\partial \vec{f}(\vec{x}(t), \vec{u}(t))}{\partial \vec{x}} \cdot \delta\vec{x} \equiv \hat{\Lambda} \cdot \delta\vec{x}, \tag{43}$$

where the inner product $(\cdot)$ is carried out between the gradient vector $\frac{\partial}{\partial \vec{x}}$ and the variation of the state vector, $\delta\vec{x}$. And $\frac{\partial \vec{f}(\vec{x}(t), \vec{u}(t))}{\partial \vec{x}}$ is the diadic tensor between the gradient $\frac{\partial}{\partial \vec{x}}$ and the vector $\vec{f}$. The matrix $\hat{\Lambda}$ is called the *Jacobian* or *Jacobi matrix* in the linear stability analysis[4, 20, 21, 23].

Next, let us define the *adjoint matrix*, $\tilde{\Lambda}$:

$$\tilde{\Lambda}_{ij} \equiv -\frac{\partial f_j(\vec{x}(t), \vec{u}(t))}{\partial x_i} = \Lambda_{ji}. \tag{44}$$

And let us define the following dynamical equations for the new functions, ψ_i:

$$\frac{d\psi_i}{dt} = -\sum_{j=1}^{n} \frac{\partial f_j(\vec{x}(t), \vec{u}(t))}{\partial x_i} \psi_j \equiv \tilde{\Lambda} \cdot \vec{\psi}, \tag{45}$$

where $\tilde{\Lambda} = -\hat{\Lambda}^{tr}$, tr meaning transpose of $\hat{\Lambda}$.

We then define the Pontryagin's Hamiltonian as

$$\mathcal{H} = \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}) = \sum_{i=1}^{n} \psi_j f_j(\vec{x}, \vec{u}). \tag{46}$$

Let us prove that the above Pontryaginian is a constant of motion in the nonlinear dynamical systems for the state variables. Please do not confuse that this problem is a problem for mechanical variables in classical mechanics. Although the Pontryagin's Hamiltonian is mathematically analogous to the Hamiltonian, it is not the same physical quantity; the former

represents the work rate (i.e., the power) and the latter the energy, as was mentioned before.

Differentiating with respect to time, we have

$$\frac{d\mathcal{H}}{dt} = \frac{d\vec{\psi}^{tr}}{dt} \cdot \vec{f}(\vec{x},\vec{u}) + \vec{\psi}^{tr} \cdot \frac{d\vec{f}(\vec{x},\vec{u})}{dt}. \tag{47}$$

Since we have

$$\frac{d\vec{f}(\vec{x},\vec{u})}{dt} = \frac{\partial \vec{f}(\vec{x},\vec{u})}{\partial \vec{x}} \cdot \dot{\vec{x}} + \frac{\partial \vec{f}(\vec{x},\vec{u})}{\partial \vec{u}} \cdot \dot{\vec{u}}, \tag{48}$$

substituting this into Eq.(47), we obtain

$$\begin{aligned}
\frac{d\mathcal{H}}{dt} &= \frac{d\vec{\psi}}{dt} \cdot \vec{f}(\vec{x},\vec{u}) + \vec{\psi} \cdot \frac{\partial \vec{f}(\vec{x},\vec{u})}{\partial \vec{x}} \cdot \dot{\vec{x}} \\
&= \frac{d\vec{\psi}^{tr}}{dt} \cdot \vec{f}(\vec{x},\vec{u}) + \vec{\psi}^{tr} \cdot \hat{\Lambda} \cdot \dot{\vec{x}} \\
&= \frac{d\vec{\psi}^{tr}}{dt} \cdot \vec{f}(\vec{x},\vec{u}) + \vec{\psi}^{tr} \cdot \hat{\Lambda} \cdot \vec{f}(\vec{x},\vec{u}) \\
&= \left(\frac{d\vec{\psi}^{tr}}{dt} + \vec{\psi}^{tr} \cdot \hat{\Lambda} \right) \cdot \vec{f}(\vec{x},\vec{u}).
\end{aligned} \tag{49}$$

Here we have assumed that the extremum condition for $\vec{f}(\vec{x},\vec{u})$ with respect to $\vec{u}$ such that

$$\frac{\partial \vec{f}(\vec{x},\vec{u})}{\partial \vec{u}} = 0. \tag{50}$$

By definition, this is equivalent to the following optimal condition:

$$\frac{\partial \mathcal{H}}{\partial \vec{u}} = 0. \tag{51}$$

Let us now impose

$$\frac{d\vec{\psi}^{tr}}{dt} + \vec{\psi}^{tr} \cdot \hat{\Lambda} = 0, \tag{52}$$

which is nothing but Eq.(45), since if we take its transpose then we have

$$\frac{d\vec{\psi}}{dt} = -\hat{\Lambda}^{tr} \cdot \vec{\psi}. \tag{53}$$

This equation is called the *adjoint equation* for the original nonlinear dynamical equations of Eq.(43). The new set of variables $\vec{\psi} = (\psi_1, \cdots, \psi_n)$ play the role of the dynamical chemical potentials of the system, which depend upon time such that the values are dynamically changing according to the control variables $\vec{u}(t) = (u_1(t), \cdots, u_m(t))$.

Substituting Eq.(52) into Eq.(49), we finally obtain

$$\frac{d\mathcal{H}}{dt} = 0. \tag{54}$$

This means that $\mathcal{H}$ is a *constant of motion*. Namely,

$$\mathcal{H} = \mathcal{W} = \text{const.} \tag{55}$$

Hence, we have proven that the Pontryagin's Hamiltonian (the Pontryaginian) is *conseved* in the course of time-development. Thus, the proof is obtained.

This Pontryaginian in the nonlienar systems with the state variables plays an important role of the Hamiltonian in classical mechanics.

D. Comparison with the Prigogine's Method

The above approach is quite analogous to the Prigogine's method in the nonlienar systems[4, 20, 21, 23]. The Prigogine's method for the stability of the nonlinear dynamics is nothing but the Liyapunov's method in mathematics.

In this method, we first assume that the left hand sides of Eq.(31) or Eq.(33) are all zeros. This provides the following:

$$\begin{cases}
0 &= f_1(x_1, \cdots, x_n, u_1, \cdots, u_m, t) \\
0 &= f_2(x_1, \cdots, x_n, u_1, \cdots, u_m, t) \\
\vdots & \qquad\qquad \vdots \\
0 &= f_n(x_1, \cdots, x_n, u_1, \cdots, u_m, t)
\end{cases}. \tag{56}$$

Solving Eq.(56) for $\vec{x}$ under fixing as $\vec{u} \equiv \vec{\lambda}$, we obtain the dynamically equilibrium states or stationary states:

$$\vec{x} = \vec{x}_{eq}. \tag{57}$$

Similar to Eq.(40), we expand the state vector as

$$\vec{x}(t) = \vec{x}_{eq} + \varepsilon \delta \vec{x}(t). \tag{58}$$

Substituting this into Eq.(33), we similarly obtain

$$\frac{d(\delta x_i)}{dt} = \sum_{j=1}^{n} \frac{\partial f_i(\vec{x}_{eq}, \vec{\lambda})}{\partial x_j} \delta x_j \equiv \sum_{j=1}^{n} \Lambda_{ij}^{eq} \delta x_j. \tag{59}$$

For the special values of $\vec{\lambda}$, we define

$$\delta x_i(t) = (\delta x_i)_{in} e^{\omega t}. \tag{60}$$

Then substituting the above into Eq.(58), we obtain

$$\omega (\delta x_i)_{in} = \sum_{j=1}^{n} \Lambda_{ij}^{eq} (\delta x_j)_{in}. \tag{61}$$

This yields the characteristic equation:

$$\left| \omega \delta_{ij} - \Lambda_{ij}^{eq} \right| = 0. \tag{62}$$

By investigating the characteristics of ω, we can find the stability condition of the equilibrium state. This approach is the essence of the Pontryagin's method. Therefore, it is nothing more than the Lyapunov method in the linear stability analysis in mathematics.

In this way, we can understand that the Pontryagin's method in the optimal control theory is a natural generalization of the Prigogine's method in nonlinear theory.

E. Generalization of the Pontryagin's Hamiltonian to the System with a Constraint

In the above, we have proven that the Pontryagin's Hamiltonian with state variables in nonlinear dynamics plays the role of the Hamiltonian of mechanical variables in classical dynamics. And we have shown that the Pontryagin's Hamiltonian is a constant of motion of the dynamical system, i.e., a conserved quantity. However, we have not yet proven that the Pontryagin's Hamiltonian takes its maximum value in the region of the admissible control parameter vectors. And we have not yet show that the principle works as well, even when there is a constraint of the system. This constraint is analogous to the constraint that we know as the *least action principle* through the Lagrangian L in classical mechanics[see Eq.(17) and Eq.(18)]. We are now going to consider these problems.

Suppose that there is a constraint in the system such as

$$\mathcal{J} = \int_{t_0}^{t_1} f_0(\vec{x}(t), \vec{u}(t), t)\, dt, \tag{63}$$

where the time-development of the system obeys Eq.(32) and Eq.(33).

Let us now impose that this constraint takes the *minimum value* in the course of the time-development of the system in between t_0 and t_1. In other words, we expect that we are able to find the control parameter vector $\vec{u}(t)$ so that always the constraint is minimized in the course of the time-development of the system in between t_0 and t_1. This simply means

$$\delta\mathcal{J} = 0. \tag{64}$$

The physical meaning of this is the following: We evaluate the functional $\mathcal{J}$ of the state variables $\vec{x}$ as if it is the action functional S in classical mechanics. Then, we expect that the value of the functional is always *minimum possible* in the course of the time-development. This constraint provides an extremum problem. In this context the functional $\mathcal{J}$ is sometimes called the *evaluation functional* or the *performance index* (PI) [8, 9]. So, we have to find the orbit of the state variables that obey the nonlinear dynamics Eq.(32) such that the PI-functional $\mathcal{J}$ must take minimum under the condition that the admissible control variables $\vec{u}$ provide the maximum for the Pontryagin's Hamiltonian. This is analogous to the least action principle for the Lagrangian under the Hamilton dynamics for mechanical variables in classical mechanics.

In this more general case than the before, we can define Pontryagin's Hamiltonian as

$$\mathcal{H} \equiv \vec{\psi}(t) \cdot \dot{\vec{x}}(t) - f_0(\vec{x}(t), \vec{u}(t), t), \tag{65}$$

$$= \vec{\psi} \cdot \vec{f}(\vec{x}, \vec{u}, t) - f_0(\vec{x}(t), \vec{u}(t), t), \tag{66}$$

$$= \sum_{j=1}^{n} \psi_j f_j(\vec{x}, \vec{u}, t) - f_0(\vec{x}(t), \vec{u}(t), t). \tag{67}$$

Obviously this has the form of the Hamiltonian in classical mechanics such as $H = \vec{p} \cdot \dot{\vec{x}} - L$.

Let us now suppose the following new variable $x_0(t)$ by

$$x_0(t) = \int_{t_0}^{t} f_0(\vec{x}(t), \vec{u}(t), t)\, dt. \tag{68}$$

By differentiation we find

$$\frac{dx_0(t)}{dt} = f_0(\vec{x}(t), \vec{u}(t), t). \tag{69}$$

Let us define a fictitious parameter

$$\psi_0 = -1. \tag{70}$$

Then we can represent the above Eq.(67) more compactly such as

$$\mathcal{H} = \sum_{j=0}^{n} \psi_j f_j(\vec{x}, \vec{u}, t). \tag{71}$$

If we read the vectors $\vec{\psi}(t)$ and $\vec{x}(t)$ in this way, it becomes the form of Eq.(34) once again.

$$\mathcal{H} = \vec{\psi}(t) \cdot \vec{f}(\vec{x}, \vec{u}, t), \tag{72}$$

where $\vec{\psi}(t) = (\psi_0(t), \psi_1(t), \cdots, \psi_n(t))$ and $\vec{f}(\vec{x}(t), \vec{u}(t), t) = (f_0(\vec{x}(t), \vec{u}(t), t), f_1(\vec{x}(t), \vec{u}(t), t), \cdots, f_n(\vec{x}(t), \vec{u}(t), t))$. However, at this time the system must obey the following nonlinear dynamics:

$$\begin{cases} \dot{x}_0 &= f_0(x_1, \cdots, x_n, u_1, \cdots, u_m, t) \\ \dot{x}_1 &= f_1(x_1, \cdots, x_n, u_1, \cdots, u_m, t) \\ \dot{x}_2 &= f_2(x_1, \cdots, x_n, u_1, \cdots, u_m, t) \\ \vdots & \qquad\qquad \vdots \\ \dot{x}_n &= f_n(x_1, \cdots, x_n, u_1, \cdots, u_m, t) \end{cases}. \tag{73}$$

As before, we then have the similar dynamics to Eq.(35) and Eq.(36):

$$\frac{d\vec{x}}{dt} = \frac{\partial\mathcal{H}}{\partial\vec{\psi}}, \tag{74}$$

$$\frac{d\vec{\psi}}{dt} = -\frac{\partial\mathcal{H}}{\partial\vec{x}}, \tag{75}$$

where $\vec{x}(t) \equiv (x_0(t), x_1(t), \cdots, x_n(t))$. Here we note that the first equaltion of Eq.(75) for ψ_0 reduces to $\dot{\psi}_0 = 0$, since $f_0(\vec{x}, \vec{u}, t)$ does not depend upon x_0 at all.

F. Pontryagin's Maximum Principle

Now we meet a very important theorem which is known as the *Pontryagin's maximum principle* in the optimal control theory[8, 9]. This theorem is described as follows:

> *Theorem 1* (Pontryagin's Maximum Principle): Let us suppose that the dynamical system is described by the nonlinear dynamical equations:
>
> $$\dot{x}_i = f_i(x_1, \cdots, x_n, u_1, \cdots, u_m, t), \tag{$M1$}$$

for $i = 0, 1, \cdots, n$.

Let $\vec{u}(t)$ be an admissible control vector in the region of U given in the time interval $t_0 \le t \le t_1$ such that the solution $\vec{x}(t)$ starts from the initial vector $\vec{x}(t_0) = \vec{x}_0$ at time t_0 and passes a point in the line Π at time t_1. Here the line Π is defined as a line that is parallel to the x_0-axis and passes the point $(0, \vec{x}_1)$ in $(n+1)$-dimensional phase space X.

One necessary condition that control $\vec{u}(t)$ and trajectory $\vec{x}(t)$ are *optimal* is that according to the functions $\vec{u}(t)$ and $\vec{x}(t)$ there must exist the following non-zero continuous vectors $\vec{\psi}(t) = (\psi_0(t), \psi_1(t), \cdots, \psi_n(t))$: (1) For all t in time interval $t_0 \le t \le t_1$, the function of variables $\vec{u}$ in the admissible region $U(\vec{u} \in U)$, $\mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u})$ takes the maximum at $\vec{u} = \vec{u}(t)$; namely,

$$\mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t), t) = \mathcal{M}(\vec{\psi}(t), \vec{x}(t), t). \qquad (M2)$$

(2) $\vec{\psi}(t)$ also satisfies the following condition:

$$\psi_0(t) = \text{const} \le 0, \qquad (M3)$$

$$\mathcal{M}(\vec{\psi}(t), \vec{x}(t), t) = \int_{t_0}^{t_1} \sum_{\alpha=0}^{n} \frac{\partial f_\alpha(\vec{x}(t), \vec{u}(t), t)}{\partial t} \psi_\alpha(t)\, dt. \qquad (M4)$$

In practice, if $\vec{\psi}(t), \vec{x}(t), \vec{u}(t)$ satisfy the coupled equations (M1) and

$$\frac{d\psi_i}{dt} = -\sum_{j=0}^{n} \frac{\partial f_j(\vec{x}(t), \vec{u}(t))}{\partial x_i} \psi_j, \qquad (M5)$$

for $i = 0, 1, \cdots, n$, and satisfy the condition (1), then the function of time t, $\psi_0(t)$, is constant, and the function $\mathcal{M}(\vec{\psi}(t), \vec{x}(t), t)$ is different from the integral of Eq.(M4) only by a constant amount. Therefore, Eq.(M4) is sufficient to be satisfied only at some instant t in $t_0 \le t \le t_1$. For example, instead of Eq.(M3) and Eq.(M4), it is sufficient if the following condition is satisfied:

$$\psi_0(t_1) \le 0, \quad \mathcal{M}(\vec{\psi}(t_1), \vec{x}(t_1), t_1) = 0. \qquad (M6)$$

The proof of the Pontryagin's maximum principle is very complicated but is given in detail in the literature[8, 9]. So, we have omitted the proof here. However, the result is quite simple enough for us to apply to physical problems.

Let us go back to the case of the nonlinear dynamics with a constraint J in §III.E. In this case, $\psi_0 = -1$ is taken. Since this is nothing but the first condition in Eq.(M6), we hold the second condition:

$$\mathcal{M}(\vec{\psi}(t_1), \vec{x}(t_1), t_1) = 0. \qquad (P1)$$

Hence, we have the following Pontryagin's maximum principle for this case: at some control vector value $\vec{u}(t) = \vec{u}$,

$$\mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t), t) = 0. \qquad (P2)$$

IV. BELLMAN'S PRINCIPLE OF OPTIMALITY AND DYNAMIC PROGRAMING

A. The Work of Richard Bellman

Richard Bellman's work in engineering mathematics and control theory has not so well-known in physics community as well[11, 12]. However, it is also very important for our purpose as well as so is Pontryagin's theory. As is shown before, on the one hand, Pontryagin's theory is the generalization of the Hamilton principle in classical mechanics to the theory of optimal control. On the other hand, Bellman's theory is the generalization of the *Hamilton-Jacobi theory* in classical mechanics to the theory of optimal control, whose theory is called the *dynamic programming* in the control theory[11, 12]. From the quality and flavor of Bellman's work and the age that the work was done, I feel like that he is "Richard Feynman"[13] in engineering mathematics. Even their faces are alike to each other as well.

B. N-stage Deterministic Process and Mathematical Representation of Policy

Let us consider the expression of the *N-stage deterministic process* in the optimal control theory and in the applied mathematics[11, 12]. It is nothing more than the *recursive processes* and the *iteration processes* in physical terminology.

Now, let us denote by a state vector $\vec{x}$ a point in an n-dimensional space. Let us denote by $\vec{u}$ the variables that we determine at each stage. Then, an N-stage deterministic process is given as follows:

$$\vec{x}_{n+1} = R(\vec{x}_n, \vec{u}_n), \quad n = 0, 1, \cdots, N, \qquad (76)$$

where we have defined $\vec{x}_0 = \vec{x}$. This produces a vector sequence:

$$[\vec{x}, \vec{x}_1, \vec{x}_2, \cdots, \vec{x}_N; \vec{u}_0, \vec{u}_1, \vec{u}_2, \cdots, \vec{u}_N]. \qquad (77)$$

Let us now define the *evaluation function* or the *performance index function* by G:

$$G(\vec{x}, \vec{x}_1, \vec{x}_2, \cdots; \vec{u}_0, \vec{u}_1, \vec{u}_2, \cdots). \qquad (78)$$

In the theory of optimal control[8, 9], the above external vector $\vec{u}$ is called the *control vector* or the *control function*. On the other hand, in the theory of dynamic programming[11, 12], it is called the *policy* or *decision*.

The evaluation function G is a function of the state vectors $\vec{x}_i$ and the policy vectors $\vec{u}_i$ from the initial state to the final state. But in order to decide the policy at any stage, the policy itself have to be evaluated by them. Therefore, the policy $\vec{q}_k$ must be thought of as a function of the past state vectors and the past policy vectors such as

$$\vec{u}_k = \vec{u}_k(\vec{x}, \vec{x}_1, \cdots, \vec{x}_k; \vec{u}_0, \vec{u}_1, \cdots, \vec{u}_{k-1}). \qquad (79)$$

This is called the *policy function*. When the policy makes the evaluation function optimal, we may call it the *optimal policy*.

And the optimality problem is that to determine the optimal policy by the multistage processes.

The above case of Eq.(79) is most general, since it includes all the information of the past. Therefore, it is very complicated, since the policies in the past determine the present policy. So, we have to simplify the policy representation by restricting ourselves to consider only the case that the state is determined by the state in the past just before the present time, such as the law of causality. In this restricted case, we have

$$\vec{u}_k = \vec{u}_k(\vec{x}_k). \tag{80}$$

Or for a bit more complicated system, it is given as

$$\vec{u}_k = \vec{u}_k(\pi_k), \tag{81}$$

where π_k is defined by

$$\pi_k = [\vec{x}_k, \vec{x}_{k-1}, \cdots]. \tag{82}$$

When we adopt the condition such as Eq.(80) or Eq.(81), the evaluation function G can be written as a sum or a product of the function of local specific variables. In this case we recognize that the *separability of the evaluation function* is realized. The evaluation function can be written in the following:

$$G = \sum_{i=0}^{N} g(\vec{x}_i, \vec{u}_i) \text{ or } G = \prod_{i=0}^{N} h(\vec{x}_i, \vec{u}_i). \tag{83}$$

$$G = \max_{0\geq i\geq N}{}^{N} h(\vec{x}_i, \vec{u}_i) \text{ or } G = \sum_{i=0}^{N-1} h(\vec{x}_i, \vec{x}_{i+1}; \vec{u}_i, \vec{u}_{i+1}). \tag{84}$$

C. Independency from the Past and Mathematical Representation of the Law of Causality

The multistage process (that is, the recursive process) always depends upon only the state one step before. Although the past, the present and the future are all connected in time series, the present state is determined by the past state one step before. This is the concept of the multistage process. Therefore, the present is nothing to do with all the past before the past one step before. In this sense, *the present is independent of the past*.

Mathematically, it is given by

$$R(\vec{x}_n) \equiv R^n(\vec{x}), \tag{85}$$

which means

$$R^N \equiv R^{N-k}(R^k). \tag{86}$$

This is the so-called mathematical representation of *the law of causality*.

We now define the mathematical representation of causality. Suppose that the state of the system is $x = f(x_0, t)$ at time t, where x_0 is the initial state of the system. Suppose that the system is progressing from the initial state $x = f(x_0, t)$ to the final state $x' = f(x_0, t + s)$ at time $t + s$.

At this moment, we can separate the whole interval from the initial time $t = 0$ to the final time $t + s$ into two intervals: one region is the interval between $t = 0$ and t and the second is the interval between t and $t + s$.

In the first interval the state lies in x_0 at time $t = 0$, and it goes to the state $x = f(x_0, t)$ at time t. In the second interval, the system is progressing from the state $x = f(x_0, t)$ at time t to the final state $x' = f(x_0, t + s)$ at time $t + s$. However, the final state is equal to the state that the system starting from the state $x = f(x_0, t)$ at time t becomes the system progressing to the state $x' = f(x, s) = f(f(x_0, t), s)$. Thus, we are able to adopt the causality condition that

$$f(x_0, t + s) = f(f(x_0, t), s). \tag{87}$$

D. Principle of Optimality and Bellman's Optimality Equation

Bellman introduced the principle of optimality[11, 12], which is described in the following principle:

> Principle of optimality:
> An optimal policy has the property that whatever the initial state and the initial decision are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision.

This principle is a very general property and has universality. And we can say that this principle of optimality is equally matched for the Dirac-Feynman's principle for the path integral in physics[13].

For example, we consider the following evaluation function:

$$G(\vec{x}, \vec{x}_1, \vec{x}_2, \cdots; \vec{u}_0, \vec{u}_1, \vec{u}_2, \cdots) = \sum_{i=0}^{N} g(\vec{x}_i, \vec{u}_i). \tag{88}$$

This is the function that this physical quantity provides data when we decide whether or not the maximum effect is attained in the multistage deterministic process. We decide whether the process is effective or not through evaluating this function. Namely, we determine so that the function becomes maximum. Therefore, we denote by $f_N(\vec{x})$ the function when it becomes maximum:

$$f_N(\vec{x}) \equiv \max_{\vec{u}_0} G(\vec{x}, \vec{x}_1, \cdots \vec{x}_N; \vec{u}_0, \vec{u}_1, \cdots, \vec{u}_N)$$

$$= \max_{\vec{u}_0} \sum_{i=0}^{N} g(\vec{x}_i, \vec{u}_i). \tag{89}$$

Since we assume that we decide the optimal policy at each step from the principle of optimality, we have

$$G_N(\vec{x}) = \sum_{i=0}^{N} g(\vec{x}_i, \vec{u}_i) = g(\vec{x}, \vec{u}_0) + [g(\vec{x}_1, \vec{u}_1) + \cdots + g(\vec{x}_N, \vec{u}_N)]$$

$$= g(\vec{x}, \vec{u}_0) + G_{N-1}(R(\vec{x}, \vec{u}_0)). \tag{90}$$

Comparing this for $N \geq 1$, we get

$$f_N(\vec{x}) = \max_{\vec{u}_0}[g(\vec{x}, \vec{u}_0) + f_{N-1}(R(\vec{x}, \vec{u}_0))]. \tag{91}$$

The initial state is defined by

$$f_0(\vec{x}) = \max_{\vec{u}_0}[g(\vec{x}, \vec{u}_0)]. \tag{92}$$

Similar functional equations are obtained for other multistage deterministic processes as well. In general we call these the *Bellman's optimality equation*.

The meaning of the principle of optimality and dynamic programming is as follows: In general, the evaluation function is a problem of the two-point boundary value of the initial and final states such that we have to consider all processes in between the interval.

In classical mechanics, we impose that the action function S becomes minimum between the initial and final states as the principle of least action. This provides the Euler-Lagrange equation for the orbit. Conversely, once the Euler-Lagrange equation is written down, we solve the Euler-Lagrange equation. This provides the temporal motion of the orbit in between the two boundary times, which guarantees that the action S becomes always minimum.

On the other hand, in the theory of optimal control, we impose that the evaluation function G becomes maximum between the initial and final states as the principle of optimality. This provides the Bellman's equation of optimality for the state. Conversely, once the Bellman's equation of optimality is written down, we solve the Bellman's equation. This provides the temporal development of the state in between the two boundary times, which guarantees that the evaluation function G becomes optimal.

In this sense, the Bellman's principle of optimality is the natural extension of the principle of least action in classical mechanics. In the automatic control engineering and the control theory, to determine the policy at each stage is called the *dynamic programming*. Bellman's dynamic programming provides algorithms to give the optimal evaluation at each stage of the process.

Inversely, we can think that the Euler-Lagrange equation of motion is the algorithm that determines the orbit of the classical object in order to give the optimal action at each time. The evaluation function in classical mechanics is the action function and the evaluation function in the optimal control theory plays the same role as the action in classical mechanics.

E. Continuous Multistage Deterministic Process

We have considered the discrete multistage deterministic processes so far. The discrete multistage deterministic processes can be generalized the *continuous multistage deterministic processes*. In this case, if we divide the time interval into very many small intervals of Δ, we can use the idea of the discrete time:

$$t = 0, \Delta, 2\Delta, \cdots. \tag{93}$$

Then we can treat the process as if it is a discrete process, and at the end we take the limit of $\Delta \to 0$.

Let us assume $N\Delta = T$. Suppose that the policy is fixed as $\vec{u}$. The transformation function $R(\vec{x}, \vec{u})$ [see Eq.(76)] is considered up to the linear term of Δ.

$$R(\vec{x}, \vec{u}) = \vec{x} + \vec{S}(\vec{x}, \vec{u})\Delta + O(\Delta^2). \tag{94}$$

The evaluation function is given by

$$G_N = \sum_{i=0}^{N} g(\vec{x}_i, \vec{u}_i)\Delta. \tag{95}$$

And we denote by f_N the maximum of the evaluation function G_N such that $f_N = \max_{\vec{u}} G_N$. Since $t = i\Delta$, we can regard it as a function of continuous time t such as $f_N = f(t)$.

We consider the evaluation function of Eq.(89) up to the linear term of Δ:

$$f_{t+\Delta}(\vec{x}) = g(\vec{x}, \vec{u})\Delta + g(R(\vec{x}, \vec{u}))\Delta + \cdots + g(R^n(\vec{x}, \vec{u}))\Delta. \tag{96}$$

Therefore, the recursive relation Eq.(90) becomes

$$f_{t+\Delta}(\vec{x}) = g(\vec{x}, \vec{u})\Delta + f_t(\vec{x} + \vec{S}(\vec{x}, \vec{u})\Delta + O(\Delta^2)). \tag{97}$$

Expanding both sides of the equation up to the linear order of Δ, and comparing the coefficients of the linear terms, we obtain the following:

$$\frac{\partial f}{\partial T} = \max_{\vec{u}}\left[g(\vec{x}, \vec{u}) + \vec{S}(\vec{x}, \vec{u}) \cdot \frac{\partial f}{\partial \vec{x}}\right]. \tag{98}$$

This is the functional equation in the continuous multistage deterministic process. This is called the *Bellman's partial differential equation*. Physically speaking, it is nothing but the Fokker-Planck equation[3] when the external force $g(\vec{x}, \vec{u})$ exists, where $\vec{S}(\vec{x}, \vec{u})$ corresponds to the velocity.

In the above we have considered the final time as a free parameter of T. However, since we can regard the initial time t_0 as a free parameter, in this case we can just replace as $dT = -dt$. Then, the corresponding equation becomes

$$\frac{\partial f}{\partial t} + \max_{\vec{u}}\left[g(\vec{x}, \vec{u}) + \vec{S}(\vec{x}, \vec{u}) \cdot \frac{\partial f}{\partial \vec{x}}\right] = 0. \tag{99}$$

This corresponds to the Hamilton-Jacobi equation in classical mechanics [see Eq.(29)], since the f and the second term in the left hand side corresponds to the action integral S and the Hamiltonian H in classical mechanics, respectively. Therefore, we cane call it the Bellman's Hamilton-Jacobi equation. This point will be discussed more explicitly later.

F. Relationship between the Variational Principle and the Dynamic Programming

At first glance, the functional equation of the dynamic programming for the continuous multistage deterministic process looks totally different from the Euler-Lagrange equation of

motion in classical mechanics. We can prove that they are equivalent to each other, however.

For the sake of simplicity, let us consider the following evaluation function with one-dimensional state vector:

$$J(x) = \int_0^T g(x, \dot{x})dt, \tag{100}$$

where $x(0) = q$. The value that the evaluation function is maximum is given by

$$f(q, T) = \max_x J(x) = \max_x \int_0^T g(x, \dot{x})dt. \tag{101}$$

The state variable is $q = x(t)$ at some fixed time t, and time left for the process becomes $T - t$. In the usual case of the variational problem, $u(t) = \dot{x}$ corresponding to the velocity(i.e., the tangent) becomes the determination of the policy.

Let us consider the problem to determine the initial tangent $\dot{x}(0)$. If we denote it by u, then the integral interval can be separated into the following two regions:

$$\int_0^T = \int_0^\Delta + \int_\Delta^T. \tag{102}$$

In the first interval,

$$\int_0^\Delta g(x, \dot{x})dt = g(q, u)\Delta + o(\Delta^2). \tag{103}$$

The principle of optimality is described as

$$f(q, T) = \max_u [g(q, u)\Delta + f(q + u\Delta, T - \Delta)] + o(\Delta^2). \tag{104}$$

Therefore, we have

$$\frac{\partial f}{\partial T} = \max_u \left[g(q, u) + u\frac{\partial f}{\partial q} \right]. \tag{105}$$

This functional relation determines both the maximum of the integral and the policy function $u = u(q, T)$.

Now, putting here $T = -t$ and calculating the right-hand side of the above equation, namely, differentiating inside [] with respect to u in order to obtain the maximum, we have

$$\frac{\partial g}{\partial u} + \frac{\partial f}{\partial q} = 0. \tag{106}$$

This is the condition to get the maximum. To satisfy the principle of optimality is to require that always this condition is satisfied. Therefore, if we think that this condition is always satisfied, then we get rid of max in the right-hand side. Hence, we have

$$\frac{\partial f}{\partial T} = -\frac{\partial f}{\partial t} = g(q, u) + u\frac{\partial f}{\partial q}. \tag{107}$$

Differentiating both sides of Eq.(132) with respect to time,

$$\frac{d}{dt}\left(\frac{\partial g}{\partial u}\right) = -\frac{d}{dt}\left(\frac{\partial f}{\partial q}\right) = -u\frac{\partial^2 f}{\partial q^2} - \frac{\partial^2 f}{\partial t \partial q}. \tag{108}$$

Similarly, differentiating both sides of Eq.(133) with respect to q,

$$\frac{\partial g}{\partial q} = -\frac{\partial f}{\partial q \partial t} - u\frac{\partial^2 f}{\partial q^2}. \tag{109}$$

Comparing both results, since each right hand side is identical, we finally obtain the Euler-Lagrange equation:

$$\frac{d}{dt}\left(\frac{\partial g}{\partial u}\right) = \frac{\partial g}{\partial q}, \quad u = \dot{q}. \tag{110}$$

In this case of the variational problem, we are not able to understand whether or not the original evaluation function takes the maximum value or the minimum value only from the extremum condition for the variation in the linear order. And the condition of Legendre is the condition that guarantees it; Namely, for the case of the maximum (minimum), we hold

$$\frac{\partial^2 g}{\partial u^2} < 0 \ (> 0). \tag{111}$$

In classical mechanics it is very difficult to put the restriction on the policy and it is not necessary to do so. However, in the dynamic programming and in the optimal control theory, there are various ranges and restrictions of the policy.

For example,

$$|u| = |\dot{x}(t)| \le k, \quad 0 \le t < T. \tag{112}$$

In such a case, since the principle of optimality is satisfied, we change the problem to the one that we seek for the maximum with a constraint. That is,

$$\frac{\partial f}{\partial T} = \max_{|u| \le k} \left[g(q, u) + u \cdot \frac{\partial f}{\partial q} \right], \quad f(q, 0) = 0. \tag{113}$$

The geometrical meaning of the dynamic programming is as follows: In classical mechanics we seek for the curve $x = x(t)$ corresponding to the orbit in the mechanical system. We select the orbit so that the action becomes maximum or minimum. Therefore, the unknown function u is regarded as a point in the functional space. On the other hand, in the dynamic programming, we seek for the optimal direction at each instant. The solution is represented by the envelope curve that is constructed by collecting the optimal directions selected at each point. Namely, it turns out to be the envelope of its tangents of the curve. Using the terminology in fluid mechanics, it corresponds to the streamline. In this respect, the variational principle in classical mechanics is dual to the principle of optimality each other. Hence, we find the duality between the variational principle and the principle of optimality.

G. Hamilton-Jacobi Equation

When we apply the principle of optimality to classical mechanics, the problem of optimal control reduces to solve the Hamilton-Jacobi equation[11, 12, 14, 15]. Consider the action integral I:

$$I = \int_{t_0}^t L(x, \dot{x}, t)dt, \tag{114}$$

where L is the Lagrangian. When the action integral takes the minimum, we write as

$$S(x_0, t_0; x, t) = \min_{\dot{x}} \int_{t_0}^{t} L(x, \dot{x}, t)dt. \tag{115}$$

Similarly as before, we divide the whole interval of time into two intervals $(t_0, t_0 + \Delta)$ and $(t_0 + \Delta, t)$:

$$S(x_0, t_0; x, t) = \min_{\dot{x}_0} \left[\int_{t_0}^{t_0+\Delta} L(x, \dot{x}, t)dt + \int_{t_0+\Delta}^{t} L(x, \dot{x}, t)dt \right]$$

$$= \min_{\dot{x}_0} [L(x, \dot{x}, t)\Delta + S(x_0 + \dot{x}_0\Delta, t_0 + \Delta; x, t)] + o(\Delta). \tag{116}$$

In the limit of $\Delta \to 0$, we have

$$\min_{\dot{x}_0} \left[L + \frac{\partial S}{\partial t_0} + \dot{x}_0 \frac{\partial S}{\partial x_0} \right] = 0. \tag{117}$$

Differentiating inside [] with respect to $\dot{x}_0$ yields

$$\frac{\partial L}{\partial \dot{x}_0} + \frac{\partial S}{\partial x_0} = 0. \tag{118}$$

And from this, we find

$$\frac{\partial L}{\partial \dot{x}_0} = -\frac{\partial S}{\partial x_0} = p_0. \tag{119}$$

p_0 is the momentum vector at $t = t_0$.

Now, this time if we apply the principle of optimality for the state x not at the initial time t_0 but at the final time t, then the terms that depend upon the time derivative change its sign to minus. Therefore, we obtain the following:

$$\min_{\dot{x}} \left[L - \frac{\partial S}{\partial t} - \dot{x} \frac{\partial S}{\partial x} \right] = 0. \tag{120}$$

$$\frac{\partial L}{\partial \dot{x}} - \frac{\partial S}{\partial x} = 0. \tag{121}$$

$$L - \dot{x} \frac{\partial S}{\partial x} - \frac{\partial S}{\partial t} = 0. \tag{122}$$

$$p \equiv \frac{\partial L}{\partial \dot{x}} = \frac{\partial S}{\partial x}. \tag{123}$$

Thus, if we define the Hamiltonian H by

$$H(x, p, t) \equiv p\dot{x} - L, \tag{124}$$

then we get

$$H\left(x, \frac{\partial S}{\partial x}, t\right) + \frac{\partial S}{\partial t} = 0. \tag{125}$$

This is again the Hamiltonian-Jacobi equation in classical mechanics.

Thus, when the idea of the Bellman's principle of optimality is applied to the special case of the action function in classical mechanics, then it reproduces to the usual the principle of least action. In this respect, the Bellman's principle of optimality is thought of as being a natural generalization of the principle of least action.

H. Relationship between the Pontryagin's Maximum Principle and the Bellman's Principle of Optimality

At the end of this section we make a comment on the relationship between the Pontryagin's maximum principle and the Bellman's principle of optimality. Although both theories seem to treat the same kind of optimal problem, the apparent looking of the results is very different. Even though we can say they are almost equivalent concepts, it is far from being trivial. Therefore, we would like to clarify this problem. This was first done by Pontryagin et al.[8, 9].

Bellman simply assume that there is a dynamical process whose the time development of the system is given by a time t in between the initial time $t = t_0$ and the final time $t = t_1$. Then, he divides the interval to two regions from $t = t_0$ to t and from t to $t = t_1$ to establish the principle of optimality. However, it is not trivial. Rather, it should be unknown till we can solve the system of nonlinear differential equations Eq.(33). In general, to solve the nonlinear equations is very difficult. Therefore, it becomes a challenging problem in physics.

Suppose that the system of the nonlinear equation of Eq.(33) would be solved under the optimal control $\vec{u}$ for $t_0 \le t \le t_1$. This gives us the time interval $T = t_1 - t_0$ as a function of the initial state of the system $\vec{x}_0$ such as

$$t_1 - t_0 = T(\vec{x}_0). \tag{126}$$

Let us define $w(\vec{x}) = -T(\vec{x}) = t - t_1$ instead of $T(\vec{x})$. For an arbitrary time t $(t_0 \le t \le t_1)$, we have

$$w(\vec{x}) = t - t_0 - T(\vec{x}_0). \tag{127}$$

Differentiating this with respect to t, we then derive the following:

$$\sum_{j=1}^{n} \frac{\partial w(\vec{x}(t))}{\partial x_j} f_j(\vec{x}(t), \vec{u}(t))$$

$$= \sum_{j=1}^{n} \frac{\partial w(\vec{x}(t))}{\partial x_j} \dot{x}_j(t) = \frac{dw(\vec{x}(t))}{dt} = 1. \tag{128}$$

For the optimal control, we have to take the optimal condition for the control parameter $\vec{u}$. So, we finally obtain the optimality relation:

$$\max_{\vec{u} \in U} \sum_{j=1}^{n} \frac{\partial w(\vec{x}(t))}{\partial x_j} f_j(\vec{x}(t), \vec{u}(t)) = 1, \tag{129}$$

where U stands for the space of admissible control. This is the result that we apply the principle of dynamic programming to the system of the nonlinear equations.

Next, let us define the function $g(\vec{x}, \vec{u})$:

$$g(\vec{x}, \vec{u}) = \sum_{j=1}^{n} \frac{\partial w(\vec{x}(t))}{\partial x_j} f_j(\vec{x}(t), \vec{u}(t)). \tag{130}$$

Differentiating this with respect x_i, we obviously find

$$\frac{\partial g(\vec{x}(t), \vec{u}(t))}{\partial x_i} = 0, \tag{131}$$

where we have used the trivial relation $g(\vec{x},\vec{u}) = 1$ by Eq.(128). After some manipulation we obtain

$$\frac{d}{dt}\left(\frac{\partial w(\vec{x}(t))}{\partial x_i}\right) = -\sum_{j=1}^{n}\frac{\partial f_j(\vec{x}(t),\vec{u}(t))}{\partial x_i}\cdot\frac{\partial w(\vec{x}(t))}{\partial x_j}. \tag{132}$$

Then, if we define

$$\psi_i(t) \equiv \frac{\partial w(\vec{x}(t))}{\partial x_i}, \;\; i = 1,\cdots,n, \tag{133}$$

then Eq.(132) turns out to be the adjoint equation:

$$\frac{d}{dt}\psi_i(t) = -\sum_{j=1}^{n}\frac{\partial f_j(\vec{x}(t),\vec{u}(t))}{\partial x_i}\cdot\psi_j(t). \tag{134}$$

On the other hand, the Eq.(129) can be written as

$$\max_{\vec{u}\in U}\sum_{j=1}^{n}\psi_j f_j(\vec{x}(t),\vec{u}(t)) = 1. \tag{135}$$

Since the left hand side of the above equation is nothing but the Pontryagin's Hamiltonian $\mathcal{H}$, hence we can prove the Pontryagin's maximum principle:

$$\mathcal{H}(\vec{\psi}(t),\vec{x}(t),\vec{u}(t)) = 1 = \mathcal{M}(\vec{\psi}(t),\vec{x}(t),\vec{u}(t)) \tag{136}$$

from using the Bellman's dynamic programming.

V. ONSAGER'S THEORY OF IRREVERSIBLE PROCESSES

A. Principle of the Least Dissipation of Energy

In the 19th century, Load Rayleigh[16] first proposed the *principle of the least dissipation of energy*, introducing the so-called *dissipation-function*. Later, this principle was fully generalized by Lars Onsager[17, 18] in the 20th century. This is simply summarized as follows.

Let us define the *dissipation-function* Φ such as

$$2\Phi(J,J) \equiv \frac{1}{T}\sum_{i,j=1}^{n}R_{ij}J_iJ_j, \tag{137}$$

where T is temperature of the system. If we define the gradient in space

$$\frac{F_i}{T} = \frac{\partial}{\partial F_i}\left(\frac{1}{T}\right) = \frac{\partial\Phi(J,J)}{\partial J_i}, \tag{138}$$

where x_1, x_2, x_3 are coordinates of three-dimensional space, then we obtain

$$2T\Phi(J,J) = T\sum_{i=1}^{3}J_i\frac{\partial\Phi(J,J)}{\partial J_i} = \sum_{i=1}^{3}J_iF_i, \tag{139}$$

where the relation between the variables F_i and J_i is given as

$$J_i = \sum_{ij}L_{ij}F_j, \tag{140}$$

$$F_i = \sum_{ij}R_{ij}J_j. \tag{141}$$

This means that the matrix L and the matrix R are inverse to each other such that $\hat{L}^{-1} = \hat{R}$ and $\hat{R}^{-1} = \hat{L}$ or $\hat{L}\hat{R} = \hat{R}\hat{L} = 1$. And Onsager found that the following relation applies for many physical systems in the linearized region in the nonlinear theory:

$$L_{ij} = L_{ji}, \;\; R_{ij} = R_{ji} \tag{142}$$

This famous relation is known as the *Onsager's reciprocal relation*. He got the Nobel Prize for this discovery.

Lord Rayleigh[16] used the function $F(J,J) = T\Phi(J,J)$ and called F the *dissipation-function*. On the other hand, Onsager[17, 18] found that $\Phi(J,J)$ is the *rate of production of entropy* due to heat flow across a volume element(of unit size) and $2T\Phi = 2F$ equals the *rate of dissipation of free energy*.

B. Variational Principle of the Least Dissipation of Energy

Following Onsager[17], the rate of local accumulation of heat eqauls

$$T\frac{ds}{dt} = -\mathrm{div}\mathbf{J} = -\frac{\partial J_1}{\partial x_1} - \frac{\partial J_2}{\partial x_2} - \frac{\partial J_3}{\partial x_3}, \tag{143}$$

where s is the local entropy density, and the total rare of increase of the S is represented by

$$\frac{dS}{dt} = \int\left(\frac{ds}{dt}\right)dV = \int\left(-\frac{1}{T}\mathrm{div}\mathbf{J}\right)dV. \tag{144}$$

By Green's formula, we can derive the following:

$$\int\int\int(-\mathrm{div}\mathbf{J})\frac{1}{T}dV + \int\int\frac{J_n}{T}d\Omega$$

$$= \int\int\int\left(\mathbf{J}, \mathrm{grad}\frac{1}{T}\right)dV$$

$$= \int\int\int\left(J_1\frac{\partial}{\partial x_1}\left(\frac{1}{T}\right) + J_2\frac{\partial}{\partial x_2}\left(\frac{1}{T}\right) + J_3\frac{\partial}{\partial x_3}\left(\frac{1}{T}\right)\right)dV, \tag{145}$$

where the double integral on the left is extended over the boundary Ω of the body in question, and J_n is the normal component of the heat flow at the boundary. If we write as

$$\dot{S}^*(J_n) \equiv \int\int\left(\frac{J_n}{T}\right)d\Omega \tag{146}$$

for the entropy given off to the surroundings, and

$$\dot{S}(J) \equiv \int\int\int\left(-\frac{1}{T}\mathrm{div}\mathbf{J}\right)dV \tag{147}$$

for the entropy change of the system proper, then we have the following:

$$\dot{S}(J) + \dot{S}^*(J_n) \equiv \int \left(\mathbf{J}, \mathrm{grad}\frac{1}{T}\right) dV \equiv \int \sum_k J_k \frac{\partial}{\partial x_k}\left(\frac{1}{T}\right) dV$$

$$\equiv \int \frac{1}{T} \sum_k J_k F_k dV, \tag{148}$$

observing Eq.(138). Now, by Eq.(138) and Eq.(139), we find

$$2\Phi(J,J) \equiv 2\int \phi(J,J) dV = \dot{S}(J) + \dot{S}^*(J_n). \tag{149}$$

By using the above preparation, we are able to show that the relations (138) are equivalent to the *variation principle*:

$$\dot{S}(J) + \dot{S}^*(J_n) - \Phi(J,J) = \text{maximum} \tag{150}$$

with the conventions that the temperature distribution $T(x_1, x_2, x_3)$ is prescribed, the flow $J(x_1, x_2, x_3)$ is varied, and the functions $\dot{S}^*$, $\dot{S}$, and Φ are defined by Eq.(146), Eq.(147), and Eq.(149), respectively. Here $\equiv$ means definition not equality. Observing Eq.(148), we have

$$\delta[\dot{S}(J) + \dot{S}^*(J) - \Phi(J,J)]$$

$$= \delta \int \left[\sum_k J_k \frac{\partial}{\partial x_k}\left(\frac{1}{T}\right) - \phi(J,J)\right] dV$$

$$= \int \sum_k \left[\frac{\partial}{\partial x_k}\left(\frac{1}{T}\right) - \frac{\partial}{\partial J_k}\phi(J,J)\right] \delta J_k dV, \tag{151}$$

so that Eq.(138) is clearly equivalent to the following:

$$\delta[\dot{S}(J) + \dot{S}^*(J_n) - \Phi(J,J)] = 0, \tag{152}$$

where since $\dot{S}$ and $\dot{S}^*$ are linear functionals of J, and Φ is a homogeneous quadratic functional, the expression in the brackets can have only one extremum. This extremum is a maximum since $\Phi(J,J)$ must be positive-definite; Otherwise, Eq.(149) would not agree with the *second law of thermodynamics*.

If the boundary is isolated the restriction

$$J_n = 0 \tag{153}$$

enters, and since then $\dot{S}^*(J_n)$ vanishes

$$\dot{S}(J) - \Phi(J,J) = \text{maximum}. \tag{154}$$

In this way, the vector J of the heat flow is described by the condition that the rate of increase of the entropy minus the dissipation-function be a maximum.

In applications, the difference between the formulations Eq.(150) and Eq.(154) is trivial. From a fundamental point of view, Eq.(154) has some merit of greater simplicity because it applies to an isolated system, and is thus more directly connected with the theory of fluctuations. Although the above result has been applied for anisotropic heat conduction, a more general theorem applying to all transport processes (conduction of electricity and heat, and diffusion) can be derived in a similar way. In this case, it is necessary to make full use of the general theory of fluctuations, involving Boltzmann's classical relation between entropy S and probability W:

$$S = k \log W + \text{const.} \tag{155}$$

This general development has been shown by Onsager and Machlup[18, 19].

C. General Principle of the Least Dissipation of Energy

Following Onsager[17], let us first denote by the variables α_i the deviations of state variables from those for the equilibrium state such that

$$\alpha_i = x_i - x_i^{eq}. \tag{156}$$

Let us introduce the *dissipation-function*:

$$\Phi(\dot{\alpha}, \dot{\alpha}) \equiv \frac{1}{2}\sum_{i,j} \rho_{ij}\dot{\alpha}_i\dot{\alpha}_j. \tag{157}$$

Therefore, $\dot{\alpha}$ describe such as J_i in Eq.(137) such that the current $J_i = \dot{\alpha}_i$ is defined by

$$J_i \equiv \dot{\alpha}_i = \sum_{j=1}^{n} G_{ij} \frac{\partial \sigma_{1\cdots n}(\alpha_1, \cdots, \alpha_n)}{\partial \alpha_j}, \quad (i = 1, \cdots, n), \tag{158}$$

where $\sigma_{1\cdots n}(\alpha_1, \cdots, \alpha_n)$ is entropy of the system, represented in terms of the language of α's. Eq.(158) is the generalization of Eq.(140).

Onsager has shown that in the approximation of the quadratic expansion of the entropy, Eq.(158) can be described by

$$F_i \equiv \frac{\partial \sigma_{1\cdots n}(\alpha_1, \cdots, \alpha_n)}{\partial \alpha_j} = \sum_{j=1}^{n} \rho_{ij} J_j, \quad (i = 1, \cdots, n), \tag{159}$$

which is the generalization of Eq.(141). So, the Onsager's reciprocal relations are given by

$$G_{ij} = G_{ji}, \quad \rho_{ij} = \rho_{ji} \tag{160}$$

And then, the description of *irreversible processes* is written by

$$\frac{\partial \sigma_{1\cdots n}}{\partial \alpha_i} = \frac{\partial \Phi(\dot{\alpha}, \dot{\alpha})}{\partial \dot{\alpha}_i}, \tag{161}$$

If we define the rate of increase of the entropy (the entropy production) as

$$\dot{S}(\alpha, \dot{\alpha}) \equiv \sum_{j=1}^{n} \frac{\partial \sigma_{1\cdots n}(\alpha_1, \cdots, \alpha_n)}{\partial \alpha_j} \dot{\alpha}_j, \quad (i = 1, \cdots, n), \tag{162}$$

then we can formulate the most general form of the variational principle:

$$\delta\left[\dot{S}(\alpha,\dot{\alpha})-\Phi(\dot{\alpha},\dot{\alpha})\right]=0. \tag{163}$$

This is derived from Eq.(161) such that

$$\delta\left[\dot{S}(\alpha,\dot{\alpha})-\Phi(\dot{\alpha},\dot{\alpha})\right]=\sum_{i=1}^{n}\left(\frac{\partial\sigma_{1\cdots n}}{\partial\alpha_i}-\frac{\partial\Phi}{\partial\dot{\alpha}_i}\right)\delta\dot{\alpha}_i=0. \tag{164}$$

Onsager called the above variational principle of Eq.(163) the *principle of the least dissipation of energy*.

In the quadratic approximation of Onsager, the dissipation-function is equal to half the rate of production of entropy:

$$2\Phi(\dot{\alpha},\dot{\alpha})=\dot{S}(\alpha,\dot{\alpha}). \tag{165}$$

This can be written as

$$\Phi(\dot{\alpha},\dot{\alpha})=\frac{1}{2}\sum_{i,j}\rho_{ij}\dot{\alpha}_i\dot{\alpha}_j=\frac{1}{2}\sum_{i,j}\dot{\alpha}_i\frac{\partial\Phi}{\partial\dot{\alpha}_i}. \tag{166}$$

Since the second law of thermodynamics

$$\dot{S}\geq 0, \tag{167}$$

$\Phi(\dot{\alpha},\dot{\alpha})$ must be *positive*. Therefore, the maximum given by Eq.(163) is always a maximum:

$$\dot{S}(\alpha,\dot{\alpha})-\Phi(\dot{\alpha},\dot{\alpha})=\text{maximum}. \tag{168}$$

This is an extension of Boltzmann's principle, which has been proven by Onsager[18, 19]. The equilibrium condition of thermodynamics:

$$S(\alpha_1,\cdots,\alpha_n)=\text{maximum} \tag{169}$$

characterizes the *most probable state*, and the probability W for an equilibrium state is given by Boltzmann's principle:

$$k\log W(\alpha_1,\cdots,\alpha_n)=S(\alpha_1,\cdots,\alpha_n)+\text{constant}. \tag{170}$$

In a similar manner, Eq.(168) describes the most probable course of an irreversible process.

The above discussion was fully generalized by Onsager and Machlup[19]. And this theory is called the *Onsager's theory of irreversible processes*[4, 20–23].

D. Least Production of Entropy for the Stationary States

The above Onsager's theory of irreversible processes[17–19] on the general principle of the least dissipation of energy was generalized by Prigogine and his coworkers[4, 20–23]. They proved a famous theorem. It was called the theorem of *principle of the least production of entropy* or the *theorem of minimum entropy production*. This theorem is described as follows.

Following the Onsager's formulation in the above, let us consider the case of two types of forces. In this case, Prigogine considered the entropy production P by

$$P\equiv\frac{dS}{dt}=\int(F_1J_1+F_2J_2)\,dV, \tag{171}$$

where F_1, F_2 stand for the forces and J_1, J_2 the corresponding currents.

Now we suppose that one component of the forces, F_1, is kept constant. In this condition, we are able to find the condition that $J_1=\text{const}$ and $J_2=0$, which means that we can find that F_2 is found to be controlled so that $J_2=0$. Since the linear phenomenological law is given by Eq.(140), we have now

$$J_1=L_{11}F_1+L_{12}F_2,\quad J_2=L_{21}F_1+L_{22}F_2, \tag{172}$$

Substituting Eq.(172) into Eq.(171), we obtain

$$P=\int\left(L_{11}F_1^2+(L_{12}+L_{21})F_1F_2+L_{22}F_2^2\right)dV. \tag{173}$$

This has a quadratic form in the integrand.

Since the entropy production P must be positive definite, the following constraints must be satisfied:

$$L_{11}>0,\quad L_{22}>0,\quad (L_{12}+L_{21})^2<4L_{11}L_{22}. \tag{174}$$

If the Onsager's reciprocal relation is satisfied, then we have

$$L_{12}=L_{21}. \tag{175}$$

This provides the condition

$$L_{12}^2<L_{11}L_{22} \tag{176}$$

and

$$P=\int\left(L_{11}F_1^2+2L_{12}F_1F_2+L_{22}F_2^2\right)dV. \tag{177}$$

When F_1 is kept constant, P can be seen as a function of F_2. By differentiating P with respect to F_2, the integral takes minimum when the following condition is satisfied

$$\frac{\partial P}{\partial F_2}=2\int(L_{12}F_1+L_{22}F_2)\,dV=0. \tag{178}$$

Thus, the entropy production P is minimum when

$$L_{12}F_1+L_{22}F_2=0 \tag{179}$$

is satisfied. That is, $P\equiv\frac{dS}{dt}$ is minimized when $J_2=0$, where J_2 is the current corresponding to the force F_2 that is not constrained to be constant. This is the theorem that when the system lies in the *stationary state*, the entropy production is minimum.

E. General Principle of the Least Production of Entropy

This argument can be analogously generalized to more general cases when many forces exist[20, 21].

Using the notations in the previous subsection, we have

$$P \equiv \frac{dS}{dt} = \int \sum_{j=1}^{n} F_i J_i dV, \tag{180}$$

where F_i stand for the generalized forces and J_i the corresponding currents. We now have to impose that

$$P > 0. \tag{181}$$

Differentiating Eq.(180) with respect to time, we have

$$\frac{dP}{dt} \equiv \int \sum_{j=1}^{n} \left(\dot{F}_i J_i + F_i \dot{J}_i \right) dV = \frac{d_F P}{dt} + \frac{d_J P}{dt}. \tag{182}$$

Here in general we can prove[4, 23]

$$\frac{d_F P}{dt} \leq 0, \tag{183}$$

while it is not necessary that we have

$$\frac{d_J P}{dt} \leq 0. \tag{184}$$

In the linear thermodynamics region, we can assume that the linear relations hold true:

$$J_i = \sum_{j=1}^{n} L_{ij} F_j, \quad F_i = \sum_{j=1}^{n} R_{ij} J_j, \tag{185}$$

where the Onsager's reciprocal relations are also assumed:

$$L_{ij} = L_{ji}, \quad R_{ij} = R_{ji}. \tag{186}$$

In this regime, we can prove that

$$\frac{d_J P}{dt} = 2 \int \sum_{i,j=1}^{n} \left(L_{ij} F_j \dot{F}_i \right) dV = \frac{d_F P}{dt} \leq 0. \tag{187}$$

Using the above, since $\frac{dP}{dt} = 2\frac{dP_F}{dt}$, we can prove

$$\frac{dP}{dt} \leq 0. \tag{188}$$

Hence, we have shown that in the linearized regime the entropy production is minimum. Thus, we are able to conclude that the least production of entropy is true in this regime.

VI. THERMODYNAMICS OF NON-EQUILIBRIUM STATES IN OPTIMAL CONTROL PROCESSES

In the Onsager's theory of irreversible processes, Onsager and Machlup[19] assumed that the quadratic nature of the dissipation-function and the entropy function such as Eq.(96). Therefore, their theory can be applied to only the linearized regime of the nonlinear equations using $\alpha_i = x_i - x_i^{eq}$. This is the weakest part of the Onsager's theory. However, their idea of the principle of the least dissipation of energy is essentially correct to the direction for taming the nonlinear problem [Eq.(32)]. We would like to solve Eq.(32) under the principle of the least dissipation of energy without using any linearization for the state variables.

A. Derivation of the Pontryagin's Hamiltonian for Thermodynamics in the Optical Processes

This can be done by using the generalized Pontryagin's Hamiltonian with a constraint described in §III.E. We do not assume any quadratic nature for the dissipation-function and entropy function at all, but we only assume that the Onsager's principle of the least dissipation of energy as a constraint in the system.

Let us regard the Onsager's variational principle for the irreversible processes as $f_0(\vec{x}(t), \vec{u}(t), t)$ in the Pontryagin's maximum principle. Let us define the following:

$$\mathcal{J} = \int_{t_0}^{t_1} f_0(\vec{x}(t), \vec{u}(t), t)\, dt$$

$$= -\int_{t_0}^{t_1} T \left[\dot{S}(\vec{x}(t), \vec{u}(t), t) - \Phi(\vec{x}(t), \vec{u}(t), t) \right] dt. \tag{189}$$

Here we have used the minus sign in front of the integral to give the least performance index under the variational principle, since the integrand provides the maximum in accordance with the maximum of Eq.(154) and Eq.(169).

The integrand $f_0(\vec{x}(t), \vec{u}(t), t)$ of Eq.(189) plays a role of Lagrangian in classical mechanics. This situation requires

$$\delta \mathcal{J} = 0. \tag{190}$$

Then, we can define the Pontryagin's Hamiltonian $\mathcal{H}$ as

$$\mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t)) \equiv \vec{\psi}(t) \cdot \dot{\vec{x}}(t) - f_0(\vec{x}(t), \vec{u}(t), t)$$

$$= \vec{\psi}(t) \cdot \vec{f}(\vec{x}, \vec{u}, t) + T \left[\dot{S}(\vec{x}(t), \vec{u}(t), t) - \Phi(\vec{x}(t), \vec{u}(t), t) \right]. \tag{191}$$

For formal understanding, let us regard $\mathcal{H}$ as $\mathcal{W} = \frac{dE}{dt} = \dot{E}$, which means the rate of internal energy increase of the system in units of Joules/sec = Watts (i.e., power). Comparing with Eq.(4), we can interpret that Eq.(191) for the non-equilibrium systems corresponds to Eq.(4) for the equilibrium systems. We can rewrite Eq.(191) such as

$$\mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t)) \equiv \mathcal{W}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t)) =$$

$$\dot{E} = \vec{\psi}(t) \cdot \dot{\vec{x}}(t) + T \left[\dot{S}(\vec{x}(t), \vec{u}(t), t) - \Phi(\vec{x}(t), \vec{u}(t), t) \right]. \tag{192}$$

Hence, we would like to note that the role of $\psi_i(t)$ ($i = 1, \cdots, n$) in the non-equilibrium thermodynamics here is that

of chemical potential μ_i ($i = 1, \cdots, n$) in the equilibrium thermodynamics.

More generally speaking, in this formalism the term of $\vec{\psi}(t)\cdot\dot{\vec{x}}(t)$ should be read as the terms of $-PdV+\sum_i F_i dx_i+\sum_j \mu_j dN_j$. For example, all of the pressure $-P$, the forces F_i, and the chemical potentials μ_i can be regarded as ψ_i's, and the volume change of the system dV, the position changes dx_i, and the number changes dN_j are regarded as $df_i(\vec{x},\vec{u},t)$'s.

Let us now compare the above Eq.(192) with Eq.(13) in the introduction. Eq.(192) contains all terms of the supply and the consumption in the equation, while Eq.(13) in thermodynamics contains only the supply by the pressure and the consumption by the entropy. Therefore, we now find that Eq.(192) is a natural extension of Eq.(13) for the equilibrium states in classical thermodynamics. Thus, we can understand that the Pontryagin's theory of optimal control is very crucial for establishing the theory of non-equilibrium thermodynamics.

B. Derivation of the Pontryagin's Equations in the optimal control processes

Now, we would like to derive the Pontryagin's Hamilton equation. Going back to Eq.(74) and Eq.(75), we assume that $\mathcal{H}$ is given by Eq.(191) and we hold

$$\frac{d\vec{x}}{dt} = \frac{\partial\mathcal{H}(\vec{\psi}(t),\vec{x}(t),\vec{u}(t))}{\partial\vec{\psi}}, \quad \frac{d\vec{\psi}}{dt} = -\frac{\partial\mathcal{H}(\vec{\psi}(t),\vec{x}(t),\vec{u}(t))}{\partial\vec{x}}, \tag{193}$$

where $\vec{x}(t) \equiv (x_1(t),\cdots,x_n(t))$, $\vec{\psi}(t) \equiv (\psi_1(t),\cdots,\psi_n(t))$, $\vec{u}(t) \equiv (u_1(t),\cdots,u_m(t))$.

The first equation in Eq.(193) provides the original nonlinear equations:

$$\frac{dx_i}{dt} = f_i(\vec{x},\vec{u},t), \quad \text{for } i = 1,\cdots,n. \tag{194}$$

On the other hand, the second equation in Eq.(194) provides

$$\frac{d\psi_i}{dt} = -\sum_{j=1}^{n}\psi_j\frac{\partial f_j(\vec{x},\vec{u})}{\partial x_i} - T\left[\frac{\partial\dot{S}(\vec{x},\vec{u})}{\partial x_i} - \frac{\partial\Phi(\vec{x},\vec{u})}{\partial x_i}\right], \tag{195}$$

for $i = 1,\cdots,n$.

We also impose the optimal condition for $\vec{u}(t)$:

$$\frac{\partial\mathcal{H}(\vec{\psi}(t),\vec{x}(t),\vec{u}(t))}{\partial u_i} = 0, \tag{196}$$

for $i = 1,\cdots,m$. This reduces to the following condition:

$$\vec{\psi}(t)\cdot\frac{\partial\vec{f}(\vec{x},\vec{u})}{\partial u_i} + T\left[\frac{\partial\dot{S}(\vec{x},\vec{u})}{\partial u_i} - \frac{\partial\Phi(\vec{x},\vec{u})}{\partial u_i}\right] = 0. \tag{197}$$

Solving this for $\vec{u}(t)$ in terms of $\vec{x}(t),\vec{\psi}(t)$, we obtain the optimal control such that $\vec{u}^o(t) \equiv \vec{u}^o(\vec{x}(t),\vec{\psi}(t))$. Substituting this into the Pontryagin's Hamiltonian $\mathcal{H}$ in Eq.(192), we obtain the optimal Pontryagin's Hamiltonian $\mathcal{H}^o \equiv \mathcal{H}^o(\vec{\psi}(t)),\vec{x}(t))$. Applying this optimal Pontryagin's Hamiltonian to the Pontryagin's equations of motion Eq.(193), we are able to obtain the optimal development of the state vector under the optimal control.

This means that under the optimal condition of Eq.(196), if the following more perticular optimal condition:

$$\frac{\partial}{\partial u_i}\left[\dot{S}(\vec{x},\vec{u}) - \Phi(\vec{x},\vec{u})\right] = 0 \tag{198}$$

is satisfied, then the Pontryagin's Hamiltonian $\mathcal{H}' \equiv \vec{\psi}(t)\cdot\vec{f}(\vec{x},\vec{u})$ must be optimal at the same time as well. In other words, under the variational principle that the dissipation of energy or the production of entropy is minimum, the Pontryagin's Hamiltonian is conserved such that it provides the maximum value as the consequence of the Pontryagin's maximum principle with a constraint.

This is the natural generalization of the extremum condition Eq.(164) [or Eq.(154)] derived by Onsager and coworker[17–19]:

$$\delta\left[\dot{S}(\vec{\alpha},\dot{\vec{\alpha}}) - \Phi(\dot{\vec{\alpha}},\dot{\vec{\alpha}})\right] = 0, \tag{199}$$

where $\vec{\alpha} = (\alpha_1,\cdots,\alpha_n)$. They considered only the cases of fluctuations of the state vectors, where the perturbed states just regress to the equilibrium state as *relaxation phenomena*. Therefore, they need not consider the nonlinear equations for the state vectors. Hence, they did not need consider the Pontryagin's Hamiltonian for the state vectors such as $\vec{\psi}\cdot\dot{\vec{\alpha}}$.

There is the main difference between our optimality condition [Eq.(197)] in this paper and the extremum condition of Onsager-Prigogine [Eq.(199)]. As is well-known, the theory of Onsager-Prigogine[17–23] is based upon the linearized regime in the nonlinear dynamics [Eq.(194)]. Therefore, it is valid only when the linear theory is applicable where the approximation of linearization $\alpha_i = x_i - x_i^{eq}$ is justified. On the other hand, our optimality condition does not require any linearizing procedure on the nonlinear dynamics, but it requires that the control variables in the original nonlinear dynamics have to be optimal. In other words, in our theory of optimal control, the control variables in the theory must be taken such that the the optimal condition of Eq.(196) or Eq.(197) is always satisfied.

Since Onsager called the above extremum condition the least dissipation of energy[17, 18], while Prigogine called it the least production of entropy[20–23], we may call our condition of Eq.(198) the *optimal dissipation of energy* or the *optimal production of entropy*.

VII. CONCLUSION

We have formulated the mathematical theory of nonequilibrium thermodynamics and thermodynamics far from equilibrium in the optimal control processes for the first time. This kind of theory has been a dream-like theory for a long time. No one simply believes that there exists such a theory that can explain thermodynamics of the very complicated nonlinear systems such as biological phenomena and the existence of life in nature. Because if such a theory exists, then we

must go beyond the standard concepts of the two laws of thermodynamics, finding a new principle in physics. However, this seems dangerous for the standard scientists who stand up on the basis.

The theory of thermodynamics started in the mid 19 century[1] and was completed in the end of the 19 century. Further through the whole 20 century, it was totally developed[2, 3]. However, this theory has to be based upon the equilibrium states of the thermal systems. Assuming the existence of equibirium state, physicists could formulate the so-called the statistical mechanics by Maxwell and Gibbs[2–4, 6]. These theories are simply called the equilibrium thermodynamics.

In nature there exist many other physical and biological phenomena that are not in the equilibrium states. In order to go beyond the equilibrium thermodynamics, Onsager[17–19, 22] succeeded to establish the theory of irreversible processes. In his theory, he generalized the principle of the least dissipation of energy originated by Lord Kelvin and Lord Rayleigh. On the other hand, Prigogine[20, 21, 23] was able to generalize the Onsager's theory of irreversible processes to the theory of the dissipative structure. In his theory, he goes forward to establish the principle of the least production of entropy.

To go further in order to understand the biological systems those theories are not sufficient enough, but there is still something missing, however. The purpose of my research has been to find such missing link between the equilibrium physical world and the actively living world.

The first hint came from the theory of electrical circuits[24]. In the electric cuircuits theory the concept of electrical power P is most important, which is measured in a unit of W (=Watts=Joules/sec). The second hint came from the theory of theoretical biology[25, 26]. In this theory, the Pontryagin's maximum theory and equivalently the Bellman's theory play an important role in the problems of theoretical biology such as plant growth etc. This gave me an impression that somehow the power is similar to the concept of Pontryagin-Bellman's theory.

Thus, I went a long journey in order to make such connections between all I need. By the intensive study for about 10 years, I found that the maximum principle of Pontryagin and the dynamic programming of Bellman are nothing but those that I have been looking for. Once this recognition is obtained, the remaining task was straightforward. The result of this effort is the present work. But this is only a beginning. Because to be able to consider the complicated biological phenomena we have to be able to treat such systems like electrical circuits. This is my dream that I left so far.

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