

Theory of Non-equilibrium Thermodynamics in the Optimal Control Processes

Part II: Physical Approaches to the Pontryagin's Maximum Principle

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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 physical meaning of the the Pontryagin's maximum principle is revealed. For this purpose, we start with the system of nonlinear differential equations $\dot{\vec{x}} = \vec{f}(\vec{x}, \vec{u}, t)$ where \vec{x} is an n -dimensional vector of state variables and \vec{u} an r -dimensional vector of control variables in the admissible control region U . We will show that when we would like to obtain the maximality of the function $\mathcal{J} = \int_{t_0}^{t_1} \mathcal{L}(\vec{x}, \vec{u}, t) dt$, where t_0, t_1 are given initial and final times, then there is a Hamiltonian $\mathcal{H} \equiv \sum_{i=1}^n \psi_i f_i(\vec{x}, \vec{u}, t) + \mathcal{L}(\vec{x}, \vec{u}, t)$, called the Pontryagin's Hamiltonian. This provides the Hamilton equations of motion for $\vec{\psi}$ and x_i : $\frac{dx_i}{dt} = \frac{\partial \mathcal{H}}{\partial \psi_i}$, $\frac{d\psi_i}{dt} = -\frac{\partial \mathcal{H}}{\partial x_i}$, with the optimality condition: $\frac{\partial \mathcal{H}}{\partial u_i} = 0$, and the maximality condition: $\frac{\partial^2 \mathcal{H}}{\partial u_i^2} \leq 0$. Thereby the Pontryagin's maximum principle is given by $\mathcal{H} \leq \max_{\vec{u} \in U} \mathcal{H} \equiv \mathcal{M} = 0$. We will apply this theory to the non-equilibrium thermodynamics in the optimal control processes, regarding $\mathcal{L}(\vec{x}, \vec{u}, t)$ as the Onsager-Prigogine's variational function such that $\mathcal{L}(\vec{x}, \vec{u}, t) = \dot{S}(\vec{x}, \vec{u}, t) - 2\Phi(\vec{x}, \vec{u}, t)$. Thus, we will show that the optimality condition for the Hamiltonian provides the concepts of the optimal dissipation of energy and the optimal production of entropy: $\sum_{i=1}^n \psi_i(t) \frac{\partial f_i(\vec{x}(t), \vec{u}(t), t)}{\partial u_s} + \frac{\partial [\dot{S}(\vec{x}, \vec{u}, t) - 2\Phi(\vec{x}, \vec{u}, t)]}{\partial u_s} = 0$, where the units of ψ_i are taken so as to adjust with the problem situation. And we show that as long as we use suitable choice for the units of the vector $\vec{\psi}$, the Pontryagin's maximum principle assures that the system realizes the energy conservation so that the power vanishes (i.e., $\mathcal{W} \equiv \frac{dE}{dt} = 0$) when the system approaches the optimal state. The proofs and the details will be discussed in this paper.

I. INTRODUCTION

A. Preliminary Motivation

In the previous paper of mine[1] we have presented the mathematical formulation for the theory of non-equilibrium thermodynamics in the optimal control processes. As the next step we would like to reformulate the same problem in terms of the more physical point of view. In this approach the theoretical framework of classical mechanics[2] will be a very nice stand point for our purpose here. Therefore, we will summarize it in the appendix.

B. Attractiveness of the Theoretical Framework of Classical Mechanics

What is most attractive in the theoretical framework of classical mechanics is as follows:

We believe that *the energy is conserved in any mechanical problem*, unless there is no dissipation of energy. This is the concept of energy conservation law. Based upon this energy conservation law, we assume that the initial energy is given in the problem for the mechanical system such as a pendulum or a spring. So, as long as there is no dissipation of energy, once the initial energy is given to the system, then it moves automatically and forever. This is our understanding on the physics of macroscopic mechanical objects.

As is described below, in classical mechanics, all variables in the system are *mechanical variables* such as the coordinates whose vector is given as \vec{x} and its momenta whose vector is given as \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 non-equilibrium thermodynamics for the systems of life or living things, the system is described by the dynamical change of the densities of ions, atoms, molecules, etc. under chemical reactions. So, the densities are given as a sum of the sets of classical particles or objects. At a given time the system is determined by the instantaneous values of the densities in the system. Since the system is dominated by the densities, we may call them the *state variables*. Thus, we have to treat the macroscopic state variables as the new type of mechanical variables in the dynamical systems.

This means that we regard the biologically living macroscopic system as a classical mechanical system given by regarding the state variables as the mechanical variables. This point of view is interesting, since we can regard the living objects such as classical mechanical objects. As a pendulum moves automatically following the energy conservation law, the macroscopic biological system moves automatically following some *unknown law of physics*. If such a new type of law exists, it will be very nice. We would like to find such new principle of conservation law. This is our goal here.

II. THE LAGRANGE'S METHOD FOR THE PONTRYAGIN'S OPTIMAL CONTROL THEORY

Now, let us start to consider the physical approaches to the *Pontryagin's theory of optimal control*[3, 4]. In other words, let us reformulate the theory from the point of view of physicists. For this purpose, we will use the standard Euler-

Lagrange's equation in classical mechanics for the system of non-linear differential equations in order to obtain the Pontryagin's theory[5–7].

A. Nonlinear Dynamical Equations of the System

In our problem here we have to consider typically the following nonlinear dynamical equations[3–7]:

$$\begin{cases} \dot{x}_1 = f_1(x_1, \dots, x_n, \lambda_1, \dots, \lambda_r, t) \\ \dot{x}_2 = f_2(x_1, \dots, x_n, \lambda_1, \dots, \lambda_r, t) \\ \vdots \\ \dot{x}_n = f_n(x_1, \dots, x_n, \lambda_1, \dots, \lambda_r, t) \end{cases} \quad (1)$$

This can be compactly written as

$$\frac{d\vec{x}}{dt} = \dot{\vec{x}} = \vec{f}(\vec{x}, \vec{\lambda}, t), \quad (2)$$

where, \vec{x} is the state vector and $\vec{\lambda}$ the externally given parameters.

This type of the equations is quite common in various theories such as theory of chemical reactions[8–12], chaos theory[13], theory of chemical oscillations[14], theory of complex systems[15], and theory of biochemical oscillations[16], etc. In these theories, we regard $\vec{\lambda}$ as constant vectors that are given initially.

On the other hand, in the optimal control theory of Pontryagin, we regard $\vec{\lambda}$ as the *control variables* in the system, however. 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:

$$\frac{d\vec{x}}{dt} = \dot{\vec{x}} = \vec{f}(\vec{x}, \vec{u}, t), \quad (3)$$

namely,

$$\begin{cases} \dot{x}_1 = f_1(x_1, \dots, x_n, u_1, \dots, u_r, t) \\ \dot{x}_2 = f_2(x_1, \dots, x_n, u_1, \dots, u_r, t) \\ \vdots \\ \dot{x}_n = f_n(x_1, \dots, x_n, u_1, \dots, u_r, t) \end{cases} \quad (4)$$

In our purpose here, we regard such state variables \vec{x} are the densities $\vec{x} \equiv (\rho_1, \dots, \rho_n)$ or concentrations $\vec{x} \equiv (N_1, \dots, N_n)$ of agents such as molecules in the system.

B. Definition of the Evaluation Function

Let us next define a function $f_0(\vec{x}(t), \vec{u}(t), t)$, and consider the following integral:

$$\mathcal{J}[\vec{x}(t), \vec{u}(t)] = \int_{t_0}^{t_1} f_0(\vec{x}(t), \vec{u}(t), t) dt, \quad (5)$$

where the state vectors in system obey Eq.(4). The functional $\mathcal{J}[\vec{x}(t), \vec{u}(t)]$ is called the *evaluation functional* or the *index of performance* (IP). According to the function f_0 , the integral measures a kind of efficiency of the system. Then, we would like to take the efficiency to be extremum – maximum or minimum such that the system would be able to perform most effectively. Therefore, we would like to impose the following condition:

$$\delta \mathcal{J}[\vec{x}(t), \vec{u}(t)] = 0. \quad (6)$$

This situation looks very similar to that in the least action principle. See Eq.(A4) and Eq.(A5) in Appendix A; $f_0(\vec{x}(t), \vec{u}(t), t)$ corresponds to the Lagrangian $L(x, \dot{x})$ in classical mechanics. Therefore, we actually regard $f_0(\vec{x}(t), \vec{u}(t), t)$ as a generalized Lagrangian that is a function of both the state vector $\vec{x}(t)$ and the control vector $\vec{u}(t)$. So, in order to make the apparent looking more similar to the Lagrangian, let us write $f_0(\vec{x}(t), \vec{u}(t), t)$ as $\mathcal{L}(\vec{x}(t), \vec{u}(t), t)$. Hence, Eq.(5) turns out to be the following:

$$\mathcal{J}[\vec{x}(t), \vec{u}(t)] = \int_{t_0}^{t_1} \mathcal{L}(\vec{x}(t), \vec{u}(t), t) dt. \quad (7)$$

C. Variational Principle and the Generalized Lagrangian

Let us consider the variational problem. We would like to find the generalized Lagrange equation of motion for our system under the constraint of the nonlinear equations of Eq.(4). Namely, we would like to find it under the constraints:

$$\vec{g}(\vec{x}, \vec{u}, t) \equiv \vec{f}(\vec{x}, \vec{u}, t) - \dot{\vec{x}} = 0. \quad (8)$$

Let us define another generalized Lagrangian \mathcal{L}' such as

$$\begin{aligned} \mathcal{L}'(\vec{x}(t), \vec{u}(t), t) &\equiv \psi_0 \mathcal{L}(\vec{x}(t), \vec{u}(t), t) + \vec{\psi}^{tr} \cdot \vec{g}(\vec{x}, \vec{u}, t) \\ &= \psi_0 \mathcal{L}(\vec{x}(t), \vec{u}(t), t) + \vec{\psi}^{tr} \cdot (\vec{f}(\vec{x}, \vec{u}, t) - \dot{\vec{x}}), \end{aligned} \quad (9)$$

where tr denotes transpose of the vector and we have defined a variable ψ_0 .

Let us first consider the Lagrange equation of motion for the state vector $\vec{x}(t)$:

$$\frac{\partial \mathcal{L}'(\vec{x}(t), \vec{u}(t), t)}{\partial \vec{x}(t)} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}'(\vec{x}(t), \vec{u}(t), t)}{\partial \dot{\vec{x}}(t)} \right) = 0. \quad (10)$$

Substituting the explicit expression of Eq.(9) into Eq.(10), we find

$$-\frac{d}{dt} \left(\frac{\partial \mathcal{L}'(\vec{x}(t), \vec{u}(t), t)}{\partial \dot{\vec{x}}(t)} \right) = \vec{\psi}^{tr}, \quad (11)$$

$$\frac{\partial \mathcal{L}'(\vec{x}(t), \vec{u}(t), t)}{\partial \vec{x}(t)} = \frac{\partial \mathcal{L}(\vec{x}(t), \vec{u}(t), t)}{\partial \vec{x}(t)} + \vec{\psi}^{tr} \cdot \frac{\partial \vec{f}(\vec{x}, \vec{u}, t)}{\partial \vec{x}(t)}, \quad (12)$$

respectively. Hence, we obtain the following equation of motion for $\vec{\psi}$:

$$\dot{\vec{\psi}}(t)^{tr} = -\frac{\partial}{\partial \vec{x}(t)} \left[\psi_0 \mathcal{L}(\vec{x}(t), \vec{u}(t), t) + \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}, t) \right]. \quad (13)$$

Let us next consider the Lagrange equation of motion for the control variables $\vec{u}(t)$:

$$\frac{\partial \mathcal{L}'(\vec{x}(t), \vec{u}(t), t)}{\partial \vec{u}(t)} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}'(\vec{x}(t), \vec{u}(t), t)}{\partial \dot{\vec{u}}(t)} \right) = 0. \quad (14)$$

Similarly, substituting the explicit expression of Eq.(9) into Eq.(14), we find

$$-\frac{d}{dt} \left(\frac{\partial \mathcal{L}'(\vec{x}(t), \vec{u}(t), t)}{\partial \dot{\vec{u}}(t)} \right) = 0, \quad (15)$$

$$\frac{\partial \mathcal{L}'(\vec{x}(t), \vec{u}(t), t)}{\partial \vec{u}(t)} = \psi_0 \frac{\partial \mathcal{L}(\vec{x}(t), \vec{u}(t), t)}{\partial \vec{u}(t)} + \vec{\psi}^{tr} \cdot \frac{\partial \vec{f}(\vec{x}, \vec{u}, t)}{\partial \vec{u}(t)}, \quad (16)$$

respectively. Hence, we obtain the following:

$$\frac{\partial}{\partial \vec{u}(t)} \left[\psi_0 \mathcal{L}(\vec{x}(t), \vec{u}(t), t) + \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}, t) \right] = 0. \quad (17)$$

In this way, the variational principle for the state vector $\vec{x}(t)$ and the control vector $\vec{u}(t)$ provides Eq.(13) and Eq.(17).

D. Pontryagin's Hamiltonian and The Equations of Motion

Let us look at Eq.(13) and Eq.(17). Both equations contain the same expression $\psi_0 \mathcal{L}(\vec{x}(t), \vec{u}(t), t) + \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}, t)$ in the []. Let us define the function:

$$\mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t), t) \equiv \psi_0 \mathcal{L}(\vec{x}(t), \vec{u}(t), t) + \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}, t). \quad (18)$$

This is called the *Pontryagin's Hamiltonian* (we would like to call *Pontryaginian*) in the theory of the optimal control[3–7]. Then, we obtain from Eq.(13)

$$\dot{\vec{\psi}}(t) = -\frac{\partial}{\partial \vec{x}(t)} \mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t), t), \quad (19)$$

and from Eq.(17)

$$\frac{\partial}{\partial \vec{u}(t)} \mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t), t) = 0, \quad (20)$$

respectively. And also we have

$$\dot{\vec{x}}(t) = \frac{\partial}{\partial \vec{\psi}(t)} \mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t), t). \quad (21)$$

Thus, we can prove the *Pontryagin's equations of motion* for \vec{x} and $\vec{\psi}$:

$$\frac{d\vec{x}}{dt} = \frac{\partial \mathcal{H}}{\partial \vec{\psi}}, \quad \frac{d\vec{\psi}}{dt} = -\frac{\partial \mathcal{H}}{\partial \vec{x}} \quad (22)$$

with a constraint for *optimality*:

$$\frac{\partial \mathcal{H}}{\partial \vec{u}} = 0. \quad (23)$$

We note that the ψ_0 comes from the situation that when we consider \mathcal{J} as a function of time t such that $\mathcal{J}(t) = \int_0^t \mathcal{L}(\vec{x}(t), \vec{u}(t), t) dt$. Hence, $\dot{\mathcal{J}} = \mathcal{L}(\vec{x}(t), \vec{u}(t), t)$. This can be seen as if we introduce one extra variable to the system, $x_0 = x_0(t)$. Therefore, we can regard $\mathcal{L}(\vec{x}(t), \vec{u}(t), t)$ as a new extra function $f_0(\vec{x}(t), \vec{u}(t), t)$ as well. Hence, we have $\dot{x}_0 = f_0(\vec{x}(t), \vec{u}(t), t)$. This can be added to the line-up in Eq.(3). Since the Hamiltonian does not include the variable x_0 , we prove $\dot{\psi}_0 = -\frac{\partial \mathcal{H}}{\partial x_0} = 0$. Hence, $\psi_0 = \text{const}$. The sign of $|\psi_0|$ depends upon the maximum or minimum principle.

Let us escape from the confusion between the standard *Hamiltonian* in classical mechanics due to Hamilton and the Pontryagin's Hamiltonian in the optimal control theory. 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*, W , [Joules/sec = Watts].

We would like to note the following: The first equation in Eq.(22) is by definition nothing but the original equations of Eq.(3). On the other hand, the second equation in Eq.(22) is something else. But it can be regarded as a generalization of the Gibbs free energy, $G = \sum_{i=1}^n \mu_i N_i$ [21].

To understand this point, let us suppose that $\mathcal{L} = 0$ and $\vec{f}(\vec{x}, \vec{u}, t)$ does not depend upon \vec{x} such as $\vec{f}(\vec{x}, \vec{u}, t) = \vec{f}(\vec{u}, t)$. In this case, Eq.(22) provides

$$\frac{d\vec{\psi}}{dt} = 0, \quad \vec{\psi} = \text{const.} \equiv \vec{\mu}. \quad (24)$$

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

$$\mathcal{H} = \vec{\mu} \cdot \dot{\vec{x}} = \vec{\mu} \cdot \vec{f}(\vec{u}, t). \quad (25)$$

The first term in Eq.(25) 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, \dots, N_n) as $\vec{x} \equiv (N_1, \dots, N_n)$ and $\vec{\mu} \equiv (\mu_1, \dots, \mu_n)$, we obtain

$$\mathcal{H} = \frac{dG}{dt} = \sum_j \mu_j \frac{dN_j}{dt} = \vec{\mu} \cdot \dot{\vec{x}}. \quad (26)$$

This expression means that the rate of Gibbs free energy \mathcal{H} is conserved under the time-development of the system. This is an indication of the existence of the dynamical relation like

$$\mathcal{W} \equiv \frac{dE}{dt} = T \frac{dS}{dt} - P \frac{dV}{dt} + \sum_i F_i \frac{dx_i}{dt} + \sum_j \mu_j \frac{dN_j}{dt}. \quad (27)$$

E. New Conservation Law

The general proof of the conservation of the Pontryagin's Hamiltonian is quite complex. We would like to present another method for this since we have already presented the proof before[1].

Differentiating the Pontryaginian \mathcal{H} with respect to time, we have

$$\frac{d\mathcal{H}}{dt} = \frac{\partial\mathcal{H}}{\partial\vec{x}} \cdot \frac{d\vec{x}}{dt} + \frac{\partial\mathcal{H}}{\partial\vec{\psi}} \cdot \frac{d\vec{\psi}}{dt} + \frac{\partial\mathcal{H}}{\partial\vec{u}} \cdot \frac{d\vec{u}}{dt}. \quad (28)$$

Next, substituting Eq.(22) and Eq.(23) into the above, we find

$$\frac{d\mathcal{H}}{dt} = \frac{\partial\mathcal{H}}{\partial\vec{x}} \cdot \frac{\partial\mathcal{H}}{\partial\vec{\psi}} + \frac{\partial\mathcal{H}}{\partial\vec{\psi}} \cdot \left(-\frac{\partial\mathcal{H}}{\partial\vec{x}}\right) = 0. \quad (29)$$

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

$$\mathcal{H} = \mathcal{W} = \text{const}. \quad (30)$$

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

This Pontryaginian with the state variables plays an important role in the nonlinear systems in the way that the Hamiltonian with mechanical variables does in classical mechanics.

F. Strategy to Solve the Problem

We have the Pontryagin's equations of motion Eq.(22) with the optimality constraint of Eq.(23). Suppose that we were able to solve Eq.(23) for the control variables \vec{u} in terms of $\vec{x}, \vec{\psi}, t$. Let us denote this by $\vec{u}^p = \vec{u}^p(\vec{x}, \vec{\psi}, t)$. Then, we substitute this into the Pontryagin's Hamiltonian \mathcal{H} . Now, we obtain

$$\mathcal{H}^o \equiv \mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}^p(\vec{x}, t), t). \quad (31)$$

At this moment, under the initial state $\vec{x}(t_0) = \vec{x}_0$ and the final state $\vec{x}(t_1) = \vec{x}_1$, the optimal orbit of the state vector and adjoint vector are given by

$$\frac{d\vec{x}}{dt} = \frac{\partial\mathcal{H}^o}{\partial\vec{\psi}}, \quad \frac{d\vec{\psi}}{dt} = -\frac{\partial\mathcal{H}^o}{\partial\vec{x}}. \quad (32)$$

G. General Optimal Control Problems

The above method can be generalized to the most general optimal control problems.

Again, let us assume that the controlled object in the system is described by the state vector \vec{x} . And the equation of the object is given by the nonlinear differential equation of Eq.(3). Then, we would like to generalize the evaluation function \mathcal{J} of Eq.(7) to the following:

$$\mathcal{J}[\vec{x}(t), \vec{u}(t)] = \int_{t_0}^{t_1} \mathcal{L}(\vec{x}(t), \vec{u}(t), t) dt + \mathcal{S}[\vec{x}(t_1), t_1], \quad (33)$$

where \mathcal{L} is the evaluation function introduced before and \mathcal{S} the final-time cost function that is the one evaluated at only the final time t_1 .

And now we impose many constraints for the control vector $\vec{u}(t)$ such that

$$g_i(\vec{u}(t)) \leq 0, \quad i = 1, \dots, r. \quad (34)$$

This set of the constraints on \vec{u} defines the control region in the control parameter space U .

For convenience, let us write Eq.(33) as

$$\mathcal{J}[\vec{x}(t), \vec{u}(t)] = \int_{t_0}^{t_1} \left[\mathcal{L}(\vec{x}(t), \vec{u}(t), t) + \frac{d\mathcal{S}(\vec{x}(t), t)}{dt} \right] dt. \quad (35)$$

By integrating the second term, we find

$$\mathcal{J}[\vec{x}(t), \vec{u}(t)] = \int_{t_0}^{t_1} \mathcal{L}(\vec{x}(t), \vec{u}(t), t) dt + \mathcal{S}[\vec{x}(t_1), t_1] - \mathcal{S}[\vec{x}(t_0), t_0]. \quad (36)$$

Since $\mathcal{S}[\vec{x}(t_0), t_0]$ at the initial time t_0 is constant by the initial condition, the terms that are important for the extremum are the first two terms. These are those in Eq.(33). So, we just leave them there in Eq.(36).

By chain rule, we find the following:

$$\frac{d\mathcal{S}(\vec{x}(t), t)}{dt} = \left[\frac{\partial\mathcal{S}(\vec{x}(t), t)}{\partial t} \right]^{tr} \cdot \dot{\vec{x}} + \frac{\partial\mathcal{S}(\vec{x}(t), t)}{\partial t}. \quad (37)$$

Therefore, the evaluation functional Eq.(35) becomes

$$\mathcal{J}[\vec{x}(t), \vec{u}(t)] =$$

$$\int_{t_0}^{t_1} \left[\mathcal{L}(\vec{x}(t), \vec{u}(t), t) + \left[\frac{\partial\mathcal{S}(\vec{x}(t), t)}{\partial t} \right]^{tr} \cdot \dot{\vec{x}} + \frac{\partial\mathcal{S}(\vec{x}(t), t)}{\partial t} \right] dt. \quad (38)$$

Now let us define the new functional $V'[\vec{x}, \vec{u},]$ such that

$$V'[\vec{x}, \vec{u}] = \int_{t_0}^{t_1} \mathcal{L}'(\vec{x}, \dot{\vec{x}}, \vec{u}, \dot{\vec{u}}, t) dt, \quad (39)$$

where we have defined as

$$\mathcal{L}'(\vec{x}, \dot{\vec{x}}, \vec{u}, \dot{\vec{u}}, t) = \mathcal{L}(\vec{x}, \vec{u}, t) + \left[\frac{\partial\mathcal{S}(\vec{x}, t)}{\partial\vec{x}} \right]^{tr} \cdot \dot{\vec{x}}$$

$$+ \frac{\partial\mathcal{S}(\vec{x}, t)}{\partial t} + \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}, t) - \vec{\psi}^{tr} \cdot \dot{\vec{x}}. \quad (40)$$

Then we would like to minimize the functional V' .

To do so, go back to the Euler-Lagarange equations, Eq.(10) and Eq.(14), once again. For \vec{x} , we have

$$\frac{\partial\mathcal{L}'(\vec{x}, \dot{\vec{x}}, \vec{u}, \dot{\vec{u}}, t)}{\partial\vec{x}} - \frac{d}{dt} \left(\frac{\partial\mathcal{L}'(\vec{x}, \dot{\vec{x}}, \vec{u}, \dot{\vec{u}}, t)}{\partial\dot{\vec{x}}} \right) = 0, \quad (41)$$

for \vec{u}

$$\frac{\partial\mathcal{L}'(\vec{x}, \dot{\vec{x}}, \vec{u}, \dot{\vec{u}}, t)}{\partial\vec{u}} - \frac{d}{dt} \left(\frac{\partial\mathcal{L}'(\vec{x}, \dot{\vec{x}}, \vec{u}, \dot{\vec{u}}, t)}{\partial\dot{\vec{u}}} \right) = 0. \quad (42)$$

Substituting the previous results into Eq.(41), we have

$$\frac{\partial}{\partial \vec{x}} \left\{ \mathcal{L}(\vec{x}, \vec{u}, t) + \left[\frac{\partial \mathcal{S}(\vec{x}, t)}{\partial \vec{x}} \right]^{tr} \cdot \dot{\vec{x}} + \frac{\partial \mathcal{S}(\vec{x}, t)}{\partial t} + \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}, t) \right\} - \frac{d}{dt} \left[\frac{\partial \mathcal{S}(\vec{x}, t)}{\partial \vec{x}} - \vec{\psi} \right] = 0. \quad (43)$$

This becomes

$$\frac{\partial}{\partial \vec{x}} \left[\mathcal{L}(\vec{x}, \vec{u}, t) + \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}, t) \right] + \left[\frac{\partial^2 \mathcal{S}(\vec{x}, t)}{\partial \vec{x}^2} \right]^{tr} \cdot \dot{\vec{x}} + \frac{\partial^2 \mathcal{S}(\vec{x}, t)}{\partial \vec{x} \partial t} - \left[\frac{\partial^2 \mathcal{S}(\vec{x}, t)}{\partial \vec{x}^2} \right]^{tr} \cdot \dot{\vec{x}} - \frac{\partial^2 \mathcal{S}(\vec{x}, t)}{\partial \vec{x} \partial t} + \dot{\vec{\psi}} = 0. \quad (44)$$

Hence, we obtain

$$\dot{\vec{\psi}} = - \frac{\partial}{\partial \vec{x}} \left[\mathcal{L}(\vec{x}, \vec{u}, t) + \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}, t) \right]. \quad (45)$$

And by similar procedure for \vec{u} we obtain

$$\frac{\partial}{\partial \vec{u}} \left[\mathcal{L}(\vec{x}, \vec{u}, t) + \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}, t) \right] = 0. \quad (46)$$

Again, we define the Pontryagin's Hamiltonian:

$$\mathcal{H} \equiv \mathcal{L}(\vec{x}, \vec{u}, t) + \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}, t). \quad (47)$$

Then we obtain the equations of motion:

$$\frac{d\vec{x}}{dt} = \frac{\partial \mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}, t)}{\partial \vec{\psi}}, \quad (48)$$

$$\frac{d\vec{\psi}}{dt} = - \frac{\partial \mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}, t)}{\partial \vec{x}}, \quad (49)$$

$$\frac{\partial \mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}, t)}{\partial \vec{u}} = 0, \quad \frac{\partial^2 \mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}, t)}{\partial \vec{u}^2} \leq 0. \quad (50)$$

In the similar way in obtaining Eq.(32), first we solve Eq.(50) for the control vector:

$$\vec{u}^o \equiv \vec{u}^o(\vec{\psi}, \vec{x}). \quad (51)$$

Next, we substitute it into the Hamiltonian such that

$$\mathcal{H}^o(\vec{\psi}, \vec{x}, t) \equiv \mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}^o(\vec{\psi}, \vec{x}), t). \quad (52)$$

Then, we are able to obtain

$$\frac{d\vec{x}}{dt} = \frac{\partial \mathcal{H}^o(\vec{\psi}, \vec{x}, \vec{u}^o, t)}{\partial \vec{\psi}}, \quad (53)$$

$$\frac{d\vec{\psi}}{dt} = - \frac{\partial \mathcal{H}^o(\vec{\psi}, \vec{x}, \vec{u}^o, t)}{\partial \vec{x}}. \quad (54)$$

H. Transversality Condition

These are very formal results, since we cannot solve them so easily unless we can specify the boundary conditions. We could solve the similar equations for the previous situation in the basic problem settings. However, in the general settings of the problem here, not only we may not know the either the initial condition or the final condition but also we may not know both at the same time. Therefore, we need more constraints for the problem to be solved.

Such an additional constraint is given by

$$\left[\frac{\partial \mathcal{L}'(\vec{x}, \dot{\vec{x}}, \vec{u}, \dot{\vec{u}}, t)}{\partial \dot{\vec{x}}} \right]^{tr} d\vec{x} \Big|_{t_1} + \left\{ \mathcal{L}'(\vec{x}, \dot{\vec{x}}, \vec{u}, \dot{\vec{u}}, t) - \left[\frac{\partial \mathcal{L}'(\vec{x}, \dot{\vec{x}}, \vec{u}, \dot{\vec{u}}, t)}{\partial \dot{\vec{x}}} \right]^{tr} \dot{\vec{x}} \right\} dt \Big|_{t_1} = 0. \quad (55)$$

This boundary condition is known as a famous condition, called the *transversality condition* in the modern control theory, where the derivation is given[3–7].

Let us calculate the above. Let us first substitute the explicit expression of Eq.(40) into $\mathcal{L}'(\vec{x}, \dot{\vec{x}}, \vec{u}, \dot{\vec{u}}, t)$. Then, we find

$$\frac{\partial \mathcal{L}'(\vec{x}, \dot{\vec{x}}, \vec{u}, \dot{\vec{u}}, t)}{\partial \dot{\vec{x}}} = \frac{\partial \mathcal{S}(\vec{x}, t)}{\partial \vec{x}} - \vec{\psi}. \quad (56)$$

Substituting Eq.(56) into Eq.(55) yields

$$\left[\frac{\partial \mathcal{S}(\vec{x}, t)}{\partial \vec{x}} - \vec{\psi} \right]^{tr} d\vec{x} \Big|_{t_1} + \left\{ \mathcal{L}(\vec{x}, \vec{u}, t) + \left[\frac{\partial \mathcal{S}(\vec{x}, t)}{\partial \vec{x}} \right]^{tr} \cdot \dot{\vec{x}} + \frac{\partial \mathcal{S}(\vec{x}, t)}{\partial t} + \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}, t) - \vec{\psi}^{tr} \cdot \dot{\vec{x}} - \left[\frac{\partial \mathcal{S}(\vec{x}, t)}{\partial \vec{x}} - \vec{\psi} \right]^{tr} \dot{\vec{x}} \right\} dt \Big|_{t_1} = 0. \quad (57)$$

This further yields

$$\left[\frac{\partial \mathcal{S}(\vec{x}, t)}{\partial \vec{x}} - \vec{\psi} \right]^{tr} d\vec{x} \Big|_{t_1} + \left[\mathcal{L}(\vec{x}, \vec{u}, t) + \vec{\psi}^{tr} \cdot \vec{f}(\vec{x}, \vec{u}, t) + \frac{\partial \mathcal{S}(\vec{x}, t)}{\partial t} \right] dt \Big|_{t_1} = 0. \quad (58)$$

Using Eq.(52), we can rewrite the adobe such as

$$\left[\frac{\partial \mathcal{S}(\vec{x}, t)}{\partial \vec{x}} - \vec{\psi} \right]^{tr} d\vec{x} \Big|_{t_1} + \left[\mathcal{H}^o(\vec{\psi}, \vec{x}, t) + \frac{\partial \mathcal{S}(\vec{x}, t)}{\partial t} \right] dt \Big|_{t_1} = 0. \quad (59)$$

This is another form of the transversality condition. We now become able to solve Eq.(53) and Eq.(54) under the condition of Eq.(59).

Let us consider the meaning of this condition. This provides us the boundary condition at the final time t_1 . Here $d\vec{x}$ and dt in the above are the difference of the position and that of time between the final position of the optimal orbit and the trajectory with taking the variation, respectively.

There are four possibilities of the condition: (1) $\vec{x}(t_1), t_1$ are all known. Therefore, $d\vec{x} = dt = 0$.; (2) $\vec{x}(t_1)$ is known but t_1 is unknown. Therefore, $d\vec{x} = 0$ but dt is arbitrary.; (3) $\vec{x}(t_1)$ is unknown but t_1 is known. Therefore, $d\vec{x}$ is arbitrary but $dt = 0$.; (4) $\vec{x}(t_1), t_1$ are all unknown. Therefore, $d\vec{x}$ and dt are all arbitrary.

For example, if condition (1) is taken, we know all boundary conditions. Therefore, we may just solve Eq.(53) and Eq.(54) at the same time under the boundary conditions.

If (4) is considered, then we are able to impose the following constraints:

$$\left[\frac{\partial \mathcal{S}(\vec{x}, t)}{\partial \vec{x}} - \vec{\psi} \right]_{t_1} = 0, \quad (60)$$

$$\left[\mathcal{H}^o(\vec{\psi}, \vec{x}, t) + \frac{\partial \mathcal{S}(\vec{x}, t)}{\partial t} \right]_{t_1} = 0. \quad (61)$$

Eq.(60) describes n equations, and of course Eq.(61) describes one equation. Hence, totally they give $n + 1$ additional constraints.

We would like to note the following: In the case of (4) the final time t_1 is unknown. Therefore, if we regard t_1 as a free parameter time t , then we have the following Hamilton-Jacobi type equations of motion for the control systems:

$$\mathcal{H}^o \left(\frac{\partial \mathcal{S}(\vec{x}, t)}{\partial \vec{x}}, \vec{x}, t \right) + \frac{\partial \mathcal{S}(\vec{x}, t)}{\partial t} = 0. \quad (62)$$

This was first obtained by Bellman and therefore was sometimes called the *Bellman's equation for the dynamic programming*[17, 18].

I. The Pontryagin's Maximum Principle

The *Pontryagin's maximum or minimum principle* is given by the optimal condition Eq.(50). It means that whatever the restrictions on the control variables \vec{u} they have to maximize or minimize the Pontryagin's Hamiltonian \mathcal{H} [3-7]. Here to be maximum or minimum depends upon whether or not we would like to maximize or minimize the Pontryagin's Hamiltonian \mathcal{H} . In other words, the control vector \vec{u} must be always determined so that the Pontryagin's Hamiltonian \mathcal{H} becomes maximum or minimum. Hence, we conclude that the optimal Pontryagin's Hamiltonian is given as

$$\begin{aligned} \mathcal{H}^o(\vec{\psi}, \vec{x}, t) &= \mathcal{H}[\vec{\psi}, \vec{x}, \vec{u}^o(\vec{\psi}, \vec{x}, t), t] \\ &= \max_{\vec{u} \in U} \mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}, t) \quad \text{or} \quad \min_{\vec{u} \in U} \mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}, t). \end{aligned} \quad (63)$$

This is the essence of the famous theorem below[3, 4]:

Theorem 1 (Pontryagin's Maximum Principle): Let us suppose that the dynamical system is described by the nonlinear dynamical equations:

$$\dot{x}_i = f_i(x_1, \dots, x_n, u_1, \dots, u_m, t), \quad (64)$$

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

Let $\vec{u}(t)$ be an admissible control vector in the region of U given in the time interval $t_0 \leq t \leq t_1$ 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 $\vec{\psi}(t) = (\psi_0(t), \psi_1(t), \dots, \psi_n(t))$:

(1) For all t in time interval $t_0 \leq t \leq t_1$, 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,

$$\mathcal{H}(\vec{\psi}(t), \vec{x}(t), \vec{u}(t), t) = \mathcal{M}(\vec{\psi}(t), \vec{x}(t), t). \quad (65)$$

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

$$\psi_0(t) = \text{const} \leq 0, \quad (66)$$

$$\mathcal{M}(\vec{\psi}(t), \vec{x}(t), t) = \int_{t_0}^{t_1} \sum_{k=0}^n \frac{\partial f_k(\vec{x}(t), \vec{u}(t), t)}{\partial t} \psi_k(t) dt. \quad (67)$$

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

$$\frac{d\psi_i}{dt} = - \sum_{j=0}^n \frac{\partial f_j(\vec{x}(t), \vec{u}(t))}{\partial x_i} \psi_j, \quad (68)$$

for $i = 0, 1, \dots, n$, 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 $t_0 \leq t \leq t_1$. For example, instead of Eq.(M3) and Eq.(M4), it is sufficient if the following condition is satisfied:

$$\psi_0(t_1) \leq 0, \quad \mathcal{M}(\vec{\psi}(t_1), \vec{x}(t_1), t_1) = 0. \quad (69)$$

III. THE VARIATIONAL METHOD FOR THE PONTRYAGIN'S OPTIMAL CONTROL THEORY

Let us next apply the variational method[6, 7] to the *Pontryagin's theory of optimal control*[3, 4] in order to understand the meaning of the Pontryagin's maximum principle more precisely.

A. Least Evaluation Function Problems

let us denote by $\vec{x} = (x_1, \dots, x_n)$ the state vector and by $\vec{u} = (u_1, \dots, u_r)$ the control vector. Again, we start with Eq.(3):

$$\dot{\vec{x}} = \vec{f}(\vec{x}, \vec{u}, t), \quad (70)$$

with the control restrictions:

$$\vec{g}(\vec{u}) \leq 0, \quad (71)$$

where $\vec{f} = (f_1, \dots, f_n)$ and $\vec{g} = (g_1, \dots, g_r)$. When the control vector has the above restrictions, it is called the *admissible control vector*.

In the optimal control problems, we have to evaluate an arbitrary functional:

$$\mathcal{J}[\vec{x}, \vec{u}] = \int_{t_0}^{t_1} \mathcal{L}(\vec{x}(t), \vec{u}(t), t) dt, \quad (72)$$

where t_0 is the initial time and t_1 the final time. Fixing the initial and final times, we would like to find the maximum or minimum of the functional, which realizes the most or least value of the evaluation functional. Since the functional fixes the both initial and final times, the problem is sometimes called the *two-point boundary value problem*.

For example, if we seek the *least time problem*, then we take $\mathcal{L} = 1$. In this case, we have

$$\mathcal{J} = \int_{t_0}^{t_1} dt = t_1 - t_0, \quad (73)$$

then we would like to seek the minimum such that

$$\min_{\vec{u}} \mathcal{J} \equiv \min_{\vec{u}} \int_{t_0}^{t_1} dt. \quad (74)$$

On the other hand, if we define a variable $x_0(t)$ such that

$$\dot{x}_0(t) = 1, \quad (75)$$

$$x_0(t) = \int_{t_0}^t dt, \quad (76)$$

then we can regard the above as one more differential equation supposed to be added to Eq.(70). In this sense we are able to generalize Eq.(70) for the n -dimensional vector to the $n + 1$ -dimensional one.

For the more general case of $\mathcal{L} (\neq 1)$, we can generalize the above discussion to

$$x_0(t) \equiv \int_{t_0}^t f_0(\vec{x}, \vec{u}, t) dt = \int_{t_0}^t \mathcal{L}(\vec{x}, \vec{u}, t) dt, \quad (77)$$

$$x_0(t_0) = 0, \quad (78)$$

which provides

$$\dot{x}_0(t) = f_0(\vec{x}, \vec{u}, t) \equiv \mathcal{L}(\vec{x}, \vec{u}, t). \quad (79)$$

Then the evaluation function becomes written as

$$x_0(t_1) = \int_{t_0}^{t_1} f_0(\vec{x}, \vec{u}, t) dt \equiv \mathcal{J}[\vec{x}, \vec{u}] = \int_{t_0}^{t_1} \mathcal{L}(\vec{x}, \vec{u}, t) dt. \quad (80)$$

Therefore, we would like to minimize or maximize the value as

$$\min_{\vec{u}} \mathcal{J} \equiv \min_{\vec{u}} x_0(t_1). \quad (81)$$

Let us note the following: For the more general cases, suppose that the new variable $x_0(t)$ is introduced by

$$x_0(t) = F(\vec{x}(t)), \quad (82)$$

where the initial condition is given by

$$x_0(t_0) = F(\vec{x}(t_0)). \quad (83)$$

Now, differentiating it with respect to time, we find

$$\dot{x}_0(t) = \sum_{k=1}^n \frac{\partial F(\vec{x})}{\partial x_k} \dot{x}_k(t) = \sum_{k=1}^n \frac{\partial F(\vec{x})}{\partial x_k} f_k(\vec{x}, \vec{u}, t). \quad (84)$$

Hence, Eq.(84) is the most general form for Eq.(75) and Eq.(79). Therefore, it is sufficient once we define the following:

$$x_0(t) = \mathcal{J}[\vec{x}, \vec{u}] = \int_{t_0}^t \mathcal{L}(\vec{x}, \vec{u}, t) dt, \quad (85)$$

$$x_0(t_0) = 0, \quad (86)$$

$$\dot{x}_0(t) = \mathcal{L}(\vec{x}, \vec{u}, t). \quad (87)$$

The functional that we have considered in the above can be considered as special cases and embedded in the more general expression for the terminal time control problem:

$$\mathcal{J} = \sum_{i=0}^n b_i x_i(t_1), \quad (88)$$

where b_i are constants. And we seek for

$$\min_{\vec{u}} \mathcal{J} = \min_{\vec{u}} \sum_{i=0}^n b_i x_i(t_1). \quad (89)$$

This type of the function is sometimes called the *Pontryagin's function* as well.

B. Maximum Principle

We would like to have the minimum or maximum of the Pontryagin's function \mathcal{J} under the certain constraints of Eq.(71) for the admissible control. Let us rewrite Eq.(88) as

$$\mathcal{J} \equiv \langle \vec{b}, \vec{x}(t_1) \rangle = \vec{b}^{tr} \cdot \vec{x}(t_1). \quad (90)$$

If we have the extremum condition:

$$\delta\mathcal{J} = 0, \quad (91)$$

then the evaluation function such as the energy or the power of the system becomes most effective, according to the contents of the system. This is the physical meaning of the maximum principle of Pontryagin. Let us prove this point.

At this time, reversely as in the previous section, let us first define the Pontryagin's Hamiltonian:

$$\mathcal{H} \equiv \langle \vec{\psi}, \vec{f} \rangle = \sum_{i=1}^n \psi_i(t) f_i(\vec{x}(t), \vec{u}(t), t), \quad (92)$$

We are going to find $\delta\mathcal{J}$ in terms of $\delta\vec{u}$ and δx_i .

Let us first consider

$$\sum_{i=1}^n \psi_i(t) \delta x_i(t) \equiv \sum_{i=1}^n \psi_i \delta x_i. \quad (93)$$

Differentiating with respect to t , we find

$$\frac{d}{dt} \left(\sum_{i=1}^n \psi_i \delta x_i \right) = \sum_{i=1}^n \dot{\psi}_i \delta x_i + \sum_{i=1}^n \psi_i \delta \dot{x}_i. \quad (94)$$

Integrate this from t_0 to t_1 . We have

$$\begin{aligned} \sum_{i=1}^n \psi_i \delta x_i \Big|_{t_0}^{t_1} &= \int_{t_0}^{t_1} \sum_{i=1}^n \dot{\psi}_i \delta x_i dt \\ &+ \int_{t_0}^{t_1} \sum_{i=1}^n \psi_i [f_i(\vec{x} + \delta\vec{x}, \vec{u} + \delta\vec{u}, t) - f_i(\vec{x}, \vec{u}, t)] dt + o(\delta x). \end{aligned} \quad (95)$$

Assuming

$$\psi_i(t_1) = -b_i, \quad \delta x_i(t_0) = 0, \quad (96)$$

we find

$$\sum_{i=1}^n \psi_i \delta x_i \Big|_{t_0}^{t_1} = - \sum_{i=1}^n b_i \delta x_i(t_1) = -\delta\mathcal{J}. \quad (97)$$

Comparing Eq.(95) with Eq.(97), we obtain

$$\begin{aligned} \delta\mathcal{J} &= - \int_{t_0}^{t_1} \sum_{i=1}^n \psi_i [f_i(\vec{x} + \delta\vec{x}, \vec{u} + \delta\vec{u}, t) - f_i(\vec{x}, \vec{u}, t)] dt \\ &\quad - \int_{t_0}^{t_1} \sum_{i=1}^n \dot{\psi}_i \delta x_i dt. \end{aligned} \quad (98)$$

Using the Taylor expansion for $f_i(\vec{x} + \delta\vec{x}, \vec{u} + \delta\vec{u}, t)$ with respect to $\delta\vec{x}$, we find

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

$$+ \frac{1}{2} \sum_{j=1}^n \sum_{k=1}^n \frac{\partial^2 f_i(\vec{x}, \vec{u} + \delta\vec{u}, t)}{\partial x_j \partial x_k} \delta x_j \delta x_k. \quad (99)$$

And we use the Pontryagin's Hamilton equation:

$$\dot{\psi}_i = - \frac{\partial \mathcal{H}}{\partial x_i} = - \sum_{j=1}^n \psi_j \frac{\partial f_j}{\partial x_i} \quad (100)$$

and Eq.(99) into Eq.(98). After some manipulation, we finally obtain the following:

$$\delta\mathcal{J} = - \int_{t_0}^{t_1} [\mathcal{H}(\vec{\psi}, \vec{x}, \vec{u} + \delta\vec{u}, t) - \mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}, t)] dt - q, \quad (101)$$

where we have defined

$$\begin{aligned} q &\equiv \int_{t_0}^{t_1} \sum_{i=1}^n \sum_{j=1}^n \psi_i \left\{ \frac{\partial [f_i(\vec{x}, \vec{u} + \delta\vec{u}, t) - f_i(\vec{x}, \vec{u}, t)]}{\partial x_j} \right\} \delta x_j dt \\ &+ \frac{1}{2} \int_{t_0}^{t_1} \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n \psi_i \frac{\partial^2 f_i(\vec{x}, \vec{u} + \delta\vec{u}, t)}{\partial x_j \partial x_k} \delta x_j \delta x_k dt + o(\delta x). \end{aligned} \quad (102)$$

The maximum principle is a *necessary condition* that the control vector \vec{u} minimizes the Pontryagin's function \mathcal{J} , i.e., $\min_{\vec{u} \in U} \mathcal{J}$ such that $\delta\mathcal{J} = 0$. To prove this the minimum condition for \mathcal{J} is never satisfied unless the Hamiltonian \mathcal{H} must be maximum. In other words, it is necessary to show that we can find at least one control vector \vec{u} that makes \mathcal{J} smaller. The condition that \mathcal{J} is minimum for any infinitesimal change $\delta\vec{u}$ of the control vector \vec{u} is the following:

$$\delta\mathcal{J} \geq 0. \quad (103)$$

Now, let us consider that the maximum principle is not satisfied in the interval (t_a, t_b) in (t_0, t_1) . Then, for an infinitesimal change $\delta\vec{u}$ of the control vector \vec{u} we have

$$\mathcal{H}(\vec{\psi}, \vec{x}, \vec{u} + \delta\vec{u}, t) - \mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}, t) \geq \alpha, \quad (104)$$

where $t_a < t < t_b$ and α is a small positive constant. In this interval $t_a < t < t_b$, only the control vector \vec{u} has a variation $\delta\vec{u}$; otherwise there is no change. Hence, we can derive the following:

$$\begin{aligned} \delta\mathcal{J} &= - \int_{t_a}^{t_b} [\mathcal{H}(\vec{\psi}, \vec{x}, \vec{u} + \delta\vec{u}, t) - \mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}, t)] dt - q, \\ &= - \int_{t_a}^{t_b} \sum_{s=1}^r \frac{\partial \mathcal{H}}{\partial u_s} \delta u_s dt - q. \end{aligned} \quad (105)$$

From Eq.(102) we see that there is δu_s in Eq.(102), too. So, we take the Taylor expansion for $f_i(\vec{x}, \vec{u} + \delta\vec{u}, t)$ in Eq.(102), again. We now have

$$f_i(\vec{x}, \vec{u} + \delta\vec{u}, t) = f_i(\vec{x}, \vec{u}, t) + \sum_{s=1}^r \frac{\partial f_i(\vec{x}, \vec{u}, t)}{\partial u_s} \delta u_s + o(\delta u_s). \quad (106)$$

Substituting this into q , we obtain

$$q = \int_{t_0}^{t_1} \sum_{i=1}^n \sum_{j=1}^n \psi_i \sum_{s=1}^r \frac{\partial^2 f_i(\vec{x}, \vec{u}, t)}{\partial x_j \partial u_s} \delta x_j \delta u_s dt. \quad (107)$$

By notifying that there is the Pontryagin's Hamiltonian inside, we obtain

$$q = \int_{t_0}^{t_1} \sum_{j=1}^n \sum_{s=1}^r \frac{\partial^2 \mathcal{H}}{\partial x_j \partial u_s} \delta x_j \delta u_s dt. \quad (108)$$

Using Eq.(108) for Eq.(105), we finally obtain the following result:

$$\delta \mathcal{J} = - \int_{t_a}^{t_b} \sum_{s=1}^r \frac{\partial \mathcal{H}}{\partial u_s} \delta u_s dt - \int_{t_0}^{t_1} \sum_{j=1}^n \sum_{s=1}^r \frac{\partial^2 \mathcal{H}}{\partial x_j \partial u_s} \delta x_j \delta u_s dt. \quad (109)$$

Therefore, if the optimality condition for the Pontryagin's Hamiltonian \mathcal{H} :

$$\frac{\partial \mathcal{H}}{\partial u_s} = 0 \quad (110)$$

is valid, then we must have the condition for the maximum:

$$\delta \mathcal{J} = 0. \quad (111)$$

Hence, the maximum principle is proved.

IV. NON-EQUILIBRIUM THERMODYNAMICS IN THE OPTIMAL CONTROL PROCESSES

A. The Principle of the Least Dissipation of Energy in Classical Mechanics

The concept of the *principle of the least dissipation of energy* was introduced by Lord Rayleigh in the 19 century[19–21]. He introduced the so-called *dissipation function* $\Phi(\vec{x}, \dot{\vec{x}}, t)$:

$$\Phi(\vec{x}, \dot{\vec{x}}, t) \equiv \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n R_{ij} \dot{x}_i \dot{x}_j \equiv \Phi(\dot{\vec{x}}), \quad (112)$$

where R_{ij} are real coefficients. Much later in 1930's Onsager found that in almost all systems :

$$R_{ij} = R_{ji}. \quad (113)$$

Since then, this relation has been called the *Onsager's reciprocal relation*.

The essence of this theory is a generalization of the Lagrange's method in classical mechanics to the one with the dissipation energy term. This theory has been applied to many areas in physics[2, 21].

As the formalism of classical mechanics is described in Appendix A, if we take the form of Lagrangian, $L(\vec{x}, \dot{\vec{x}})$, then we find the following Euler-Lagrange's equation of motion:

$$\frac{d}{dt} \left(\frac{\partial L(\vec{x}, \dot{\vec{x}})}{\partial \dot{\vec{x}}} \right) - \frac{\partial L(\vec{x}, \dot{\vec{x}})}{\partial \vec{x}} = - \frac{\partial \Phi(\dot{\vec{x}})}{\partial \dot{\vec{x}}} \equiv \vec{Q}(\dot{\vec{x}}), \quad (114)$$

where $\vec{F}(\dot{\vec{x}})$ is the damping force or the dissipative force defined by

$$\vec{Q}(\dot{\vec{x}}) \equiv - \frac{\partial \Phi(\dot{\vec{x}})}{\partial \dot{\vec{x}}}. \quad (115)$$

Therefore, the work W done by this force is given by

$$\begin{aligned} W &= \vec{Q}(\dot{\vec{x}})^T \dot{\vec{x}} = \sum_{i=1}^n Q_i \dot{x}_i \\ &= - \sum_{i=1}^n \sum_{j=1}^n R_{ij} \dot{x}_i \dot{x}_j = -2\Phi. \end{aligned} \quad (116)$$

Now, defining the kinetic energy $T(\dot{\vec{x}})$ and the potential energy $U(\vec{x})$, we adopt the Lagrangian:

$$L(\vec{x}, \dot{\vec{x}}) = T(\dot{\vec{x}}) - U(\vec{x}). \quad (117)$$

Applying this into Eq.(11), we obtain

$$\frac{dp_i}{dt} = - \frac{\partial U(\vec{x})}{\partial x_i} - \frac{\partial \Phi(\dot{x}_i)}{\partial \dot{x}_i}, \quad (118)$$

$$\frac{dx_i}{dt} = \frac{\partial T(\vec{p})}{\partial p_i}, \quad p_i = \frac{\partial T(\dot{\vec{x}})}{\partial \dot{x}_i}. \quad (119)$$

We now are able to calculate the energy conservation law with the energy dissipation as follows:

$$\begin{aligned} \frac{dH}{dt} &= \frac{d}{dt}(T + U) = \sum_{i=1}^n \left(\frac{\partial T}{\partial p_i} \dot{p}_i + \frac{\partial U}{\partial x_i} \dot{x}_i \right) \\ &= \sum_{i=1}^n \left(\dot{p}_i + \frac{\partial U}{\partial x_i} \right) \dot{x}_i. \end{aligned} \quad (120)$$

Substituting Eq.(118) into the above, we obtain

$$\frac{dH}{dt} = - \sum_{i=1}^n \frac{\partial \Phi(\dot{x}_i)}{\partial \dot{x}_i} \dot{x}_i = \sum_{i=1}^n Q_i \dot{x}_i = -2\Phi. \quad (121)$$

Hence, we are led to the following conservation law for the dissipative systems:

$$W = \frac{dH}{dt} = -2\Phi. \quad (122)$$

When we have an external force F_i from the outside of the system, then it will be

$$W = \frac{dH}{dt} = P_{ex} - 2\Phi, \quad (123)$$

where P_{ex} means the power of the power source from the outside of the system,

$$P_{ex} = \sum_{i=1}^n F_i \dot{x}_i. \quad (124)$$

Thus, the energy conservation occurs only when no outside power $P_{ex} = 0$ source and no dissipation $D = 0$ such that

$$W = \frac{dH}{dt} = 0. \quad (125)$$

This is the theory of dissipation of energy in classical mechanics.

B. The Principle of the Least Dissipation of Energy in Thermodynamics

Onsager[22–27] generalized this idea to the systems of irreversible processes in thermodynamics, where the variables are turned out to be *state* variables, not *mechanical* variables, contrary to classical mechanics.

Main clue to do this was to specify the generalized forces X_i in terms of entropy. Suppose that S is the entropy of the system. Then, the generalized force X_i is defined by

$$X_i = \frac{\partial S}{\partial x_i}. \quad (126)$$

This relies upon a simple observation that in most of irreversible processes the equations of motion is described by a relaxation equation or a damping equation:

$$\dot{x}_i = f_i(x_1, \dots, x_n) = - \sum_{k=1}^n \lambda_{ik} x_k, \quad (127)$$

where we would like to note that they are *linear* equations.

On the other hand, using the Boltzmann's principle:

$$S = k_B \log W, \quad (128)$$

where k_B is the Boltzmann constant, and using the Einstein's principle for entropy fluctuations around an *equilibrium* state, the entropy function S can be expanded as

$$S = S_0 - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n s_{ij} x_i x_j. \quad (129)$$

Applying this for Eq.(126), we obtain

$$X_i = - \sum_{k=1}^n s_{ik} x_k. \quad (130)$$

If we notify x_i in Eq.(127) and Eq.(130) to describe the fluctuations from the equilibrium state such that $\alpha_i \equiv x_i - x_i^{(0)}$, then we have

$$\dot{\alpha}_i = - \sum_{k=1}^n \lambda_{ik} \alpha_k, \quad (131)$$

$$X_i = - \sum_{k=1}^n s_{ik} \alpha_k = \sum_{k=1}^n R_{ik} \dot{\alpha}_k. \quad (132)$$

Comparing this with Eq.(127), it gives $\lambda_{ij} = \sum_{k=1}^n (R^{-1})_{ik} s_{kj} = (R^{-1} s)_{ij}$. Eliminating $\alpha_k (k = 1, \dots, n)$ from Eq.(131) and Eq.(132), we find

$$J_i \equiv \dot{\alpha}_i = \sum_{k=1}^n L_{ik} X_k, \quad (133)$$

where

$$L_{ij} = \sum_{k=1}^n \lambda_{ik} (s^{-1})_{kj} = (R^{-1})_{ij} = L_{ji}. \quad (134)$$

In the linearized level, we can do the similar thing for the equation of motion for X_i conjugate to Eq.(133) and then we obtain

$$\dot{X}_i = \sum_{k=1}^n \zeta_{ik} \alpha_k, \quad (135)$$

where

$$\zeta_{ij} = \sum_{k=1}^n s_{ik} \lambda_{kj} = \sum_{k=1}^n \sum_{l=1}^n s_{ik} L_{kl} s_{lj} = \zeta_{ji}. \quad (136)$$

Now, Eq.(133) can be rewritten as

$$\dot{\alpha}_i = \frac{\partial \Phi}{\partial X_i}, \quad (137)$$

$$\Phi = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n L_{ij} X_i X_j. \quad (138)$$

From the function D together with Eq.(126) and Eq.(137), we can calculate the rate of entropy production \dot{S} as

$$\sigma \equiv \dot{S} = \sum_{i=1}^n \frac{\partial S}{\partial \alpha_i} \dot{\alpha}_i = \sum_{i=1}^n X_i \dot{\alpha}_i = \sum_{i=1}^n X_i \frac{\partial \Phi}{\partial X_i}. \quad (139)$$

Since $\sum_{i=1}^n X_i \frac{\partial D}{\partial X_i} = 2\Phi$, hence, we obtain

$$\sigma \equiv \dot{S} = 2\Phi. \quad (140)$$

Analogously we obtain

$$\dot{X}_i = \frac{\partial \Phi}{\partial \alpha_i}, \quad (141)$$

$$\Phi = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \zeta_{ij} \alpha_i \alpha_j. \quad (142)$$

And hence, we have

$$\sigma \equiv \dot{S} = \sum_{i=1}^n \alpha_i \dot{X}_i = 2\Phi. \quad (143)$$

Thus, there is duality between the state variables α_i (or x_i) and the generalized forces X_i .

The similarity between Eq.(122) for the work rate W in classical mechanics and Eq.(140) for the entropy production in thermodynamics is very impressive. So, Onsager[21–27] named this by the *principle of the least production of entropy* for thermodynamics.

Following the above Onsager's method, Landau[21] continued the argument further to thermodynamic systems. Suppose that R_{min} is the minimum work needed to bring the system from the equilibrium state to the present state. Then, the entropy change in a closed system is given by

$$\Delta W = - \frac{R_{min}}{T_0}. \quad (144)$$

If we put

$$R_{min} = \Delta E - T_0 \Delta S + P_0 \Delta V, \quad (145)$$

where E, S, V are thermodynamic quantities for the closed system and T_0, P_0 are the temperature and pressure for the medium. Thus, we obtain

$$\dot{E} - T_0 \dot{S} + P_0 \dot{V} = -2T_0 \Phi. \quad (146)$$

If we use the Gibbs' free energy: $G = E - TS + PV = F + PV$, assuming $T = T_0, P = P_0$, then we obtain

$$\dot{G} = -2T\Phi. \quad (147)$$

If the system is at constant pressure and volume, then we finally obtain

$$\dot{F} = -2T\Phi, \text{ or } \frac{\dot{F}}{T} = -2\Phi, \quad (148)$$

where F is the Helmholtz's free energy. This is nothing but the thermodynamics version of the principle of the least dissipation of energy, obtained from the principle of the least production of entropy.

Analogous to Eq.(123), if there is an external thermal source Q_i that can either heat up or cool down the system, then Eq.(148) turns out to be the following: If the system is at constant pressure and volume, then we finally obtain

$$\dot{F} = TP_{ex} - 2T\Phi, \text{ or } \frac{\dot{F}}{T} = P_{ex} - 2\Phi, \quad (149)$$

where P_{ex} means the power of the thermal source from the outside of the system,

$$P_{ex} = \frac{1}{T} \sum_{i=1}^n Q_i \dot{\alpha}_i. \quad (150)$$

In this way, the principle of the least dissipation of energy and the principle of the least generation of entropy are very elegantly combined together to be embedded in a unified theory in equilibrium thermodynamics. However, it can be done only in the level: (a) The *linearized* theory is valid as approximation; (b) All deviations of the state variables are located near the equilibrium state; (c) Furthermore, as is implemented in the Einstein's theory of fluctuations, there is an implicit assumption that the equilibrium state has already accomplished the maximum of the system.

These are the points that we would like to generalize to any thermodynamic systems far from equilibrium and to the non-linear theory. This seems to be carried out by the theory of optimal control processes in the previous sections.

C. The Principle of the Least Production of Entropy in Thermodynamics

As is discussed in the previous sections, we have understood the physical meaning of the Pontryagin's maximum

principle in the optimal control processes. Let us now use the maximum principle to the theory of classical thermodynamics. In this case, we have to be able to specify which is which. Namely, we have to answer what is supposed to be \mathcal{J} and what is to be \mathcal{H} as well as \mathcal{L} .

Recently Iguchi has presented such ideas for the first time[1]. He postulated that the evaluation functional for the thermodynamics is nothing more than the famous entropy production in terms of the language of the Onsager-Prigogine's theory of irreversible processes[8–12, 22–27].

To know more precisely this point, let us go back to Eq.(140) and we rewrite it as

$$\dot{S}(\vec{\alpha}) - 2\Phi(\vec{\alpha}) = 0, \quad (151)$$

where $\sigma = \dot{S}$. Onsager noticed that this can be understood as a special case of the following more general condition:

$$\dot{S}(\vec{\alpha}) - 2\Phi(\vec{\alpha}) = \text{maximum}. \quad (152)$$

This is valid for the irreversible processes from the equilibrium, where at the equilibrium state we must keep the condition for thermodynamic equilibrium:

$$S(\vec{\alpha}) = \text{maximum}. \quad (153)$$

The Gibbs' theory for the thermal equilibrium state starts from the condition of Eq.(153)[21], while the Onsager's theory for the non-equilibrium near the equilibrium state starts from the condition Eq.(152)[22–27].

The meaning of Eq.(152) as well as Eq.(153) is that the problem here is a variational problem. Therefore, to be able to reach the maximum we have to consider the variational problem taking its extremum condition:

$$\delta[\dot{S}(\vec{\alpha}) - 2\Phi(\vec{\alpha})] = 0 \text{ for the irreversible state}, \quad (154)$$

$$\delta[S(\vec{\alpha})] = 0 \text{ for the equilibrium state}, \quad (155)$$

respectively.

This theory has been generalized by Onsager and Machlup[26, 27] to more general cases where the entropy function is a function of α_i and $\dot{\alpha}_i$ such that $S = S(\vec{\alpha}, \dot{\vec{\alpha}})$. In this case, Eq.(126) is generalized to the following:

$$X_i \equiv \frac{\partial S(\vec{\alpha}, \dot{\vec{\alpha}})}{\partial \alpha_i} + \frac{d}{dt} \left(\frac{\partial S(\vec{\alpha}, \dot{\vec{\alpha}})}{\partial \dot{\alpha}_i} \right) \equiv \sum_{k=1}^n R_{ik} \dot{\alpha}_k. \quad (156)$$

And the entropy is expanded as

$$S = S_0 - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n s_{ij} \alpha_i \alpha_j - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n m_{ij} \dot{\alpha}_i \dot{\alpha}_j. \quad (157)$$

Then, substituting Eq.(157) into eq.(156), we obtain the following instead of Eq.(131):

$$\sum_{k=1}^n (m_{ik} \ddot{\alpha}_k + R_{ik} \dot{\alpha}_k + s_{ik} \alpha_k) = 0. \quad (158)$$

Using this together with Eq.(156), we can derive the following relation for the entropy production:

$$\begin{aligned}\dot{S} &= - \sum_{i=1}^n \sum_{j=1}^n s_{ij} \alpha_i \dot{\alpha}_j - \sum_{i=1}^n \sum_{j=1}^n m_{ij} \dot{\alpha}_i \ddot{\alpha}_j \\ &= - \sum_{i=1}^n \sum_{j=1}^n (s_{ij} \alpha_i + m_{ij} \ddot{\alpha}_j) \dot{\alpha}_i = \sum_{i=1}^n X_i \dot{\alpha}_i \\ &= 2\Phi(\dot{\alpha}, \dot{\alpha}) = 2\Psi(\vec{X}, \vec{X}),\end{aligned}\quad (159)$$

where we have defined as

$$\Phi(\dot{\alpha}, \dot{\alpha}) = \frac{1}{2} \dot{\alpha}^T R \dot{\alpha}, \quad \Psi(\vec{X}, \vec{X}) = \frac{1}{2} \vec{X}^T L \vec{X}, \quad (160)$$

where $L = R^{-1}$. Hence, we are also led to the following extremum condition:

$$\int_{t_0}^{t_1} [\dot{S}(\dot{\alpha}, \dot{\alpha}) - 2\Phi(\dot{\alpha}, \dot{\alpha}) - 2\Psi(\vec{X}, \vec{X})] dt = \text{maximum}. \quad (161)$$

Thus, Onsager and Machlup[26, 27] have concluded that if we regard the integrand as a Lagrangian:

$$\mathcal{L}(\dot{\alpha}, \dot{\alpha}, \ddot{\alpha}) = \dot{S}(\dot{\alpha}, \dot{\alpha}) - 2\Phi(\dot{\alpha}, \dot{\alpha}) - 2\Psi(\vec{X}, \vec{X}), \quad (162)$$

then we can use the variational method to the irreversible processes as well. In fact, applying the Euler-Lagrange's equation:

$$\frac{d^2}{dt^2} \left(\frac{\partial \mathcal{L}}{\partial \ddot{\alpha}_i} \right) - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\alpha}_i} \right) + \frac{\partial \mathcal{L}}{\partial \alpha_i} = 0, \quad (i = 1, \dots, n), \quad (163)$$

we obtain the equations of motion Eq.(158) of the system, once again. Thus, the processes of damping or relaxation in the irreversible processes realize the maximum principle in this sense.

D. The Principle of the Least Production of Entropy

Prigogine[8–12] has generalized the above Onsager's theory in the irreversible processes to the theory of dissipative structure. As was shown before, Onsager has concentrated only on the relaxation phenomena that the fluctuations go back to the equilibrium state, where the equations of motion are given by Eq.(158). On the contrary, Prigogine has started with the nonlinear equations:

$$\begin{cases} \dot{x}_1 = f_1(x_1, \dots, x_n, \lambda_1, \dots, \lambda_r, t) \\ \dot{x}_2 = f_2(x_1, \dots, x_n, \lambda_1, \dots, \lambda_r, t) \\ \vdots \\ \dot{x}_n = f_n(x_1, \dots, x_n, \lambda_1, \dots, \lambda_r, t) \end{cases} \quad (2)$$

Here, $\vec{x} = (x_1, \dots, x_n)$ is the state vector and $\vec{\lambda} = (\lambda_1, \dots, \lambda_r)$ the vector with the external parameters, where

$\vec{f} = (f_1, \dots, f_n)$ can be nonlinear functions. This type of the equations is quite common in various theories[8–16].

In this method, we first assume that the left hand sides of Eq.(2) are all zeros such that

$$\begin{cases} 0 = f_1(x_1, \dots, x_n, \lambda_1, \dots, \lambda_r, t) \\ 0 = f_2(x_1, \dots, x_n, \lambda_1, \dots, \lambda_r, t) \\ \vdots \\ 0 = f_n(x_1, \dots, x_n, \lambda_1, \dots, \lambda_r, t) \end{cases} \quad (164)$$

Solving Eq.(164) for \vec{x} , we obtain the dynamically equilibrium states or stationary states in terms of $\vec{\lambda}$:

$$\vec{x} = \vec{x}_{eq}(\vec{\lambda}) \equiv \vec{x}_{eq}. \quad (165)$$

Now, we expand the state vector as

$$\vec{x}(t) = \vec{x}_{eq} + \varepsilon \delta \vec{x}(t). \quad (166)$$

Substituting this into Eq.(2), we obtain

$$\frac{d(\delta x_i)}{dt} = \sum_{j=1}^n \frac{\partial f_i(\vec{x}_{eq}, \vec{\lambda})}{\partial x_j} \delta x_j \equiv \sum_{j=1}^n \Lambda_{ij}^{eq} \delta x_j. \quad (167)$$

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

$$\delta x_i(t) = (\delta x_i)_{in} e^{\omega t}. \quad (168)$$

Then substituting Eq.(168) into Eq.(167), we obtain

$$\omega(\delta x_i)_{in} = \sum_{j=1}^n \Lambda_{ij}^{eq} (\delta x_j)_{in}. \quad (169)$$

This yields the characteristic equation:

$$|\omega \delta_{ij} - \Lambda_{ij}^{eq}| = 0. \quad (170)$$

By investigating the characteristics of ω , we can find the stability condition of the equilibrium state: If all ω_i ($i = 1, \dots, n$) are negative real then the system is stable.

Please note here that the above equilibrium state of Prigogine is not the thermally equilibrium state treated by Gibbs and Onsager. The former is the *dynamical equilibrium* such as chemical equilibrium, while the latter is the *static equilibrium* in the usual sense of thermodynamics where the entropy S is maximum. So, Prigogine generalized the idea of Onsager to the systems of the dynamical equilibrium state. In fact, this can be done by regarding Onsager's fluctuations $\alpha_i = x_i - x_0$ which are the deviations from the thermal equilibrium as the dynamical fluctuations $\alpha_i = x_i - x_{eq}(\lambda)$ which are the deviations from the dynamical equilibrium.

Once we recognize this correspondence, we use the Onsager's approach discussed before. Therefore, Prigogine used Onsager's theory to the systems of the dynamical equilibrium state, making the analogy between the fluctuations from the thermal equilibrium and the fluctuations from the dynamical equilibrium.

Let us define the entropy S by

$$S \equiv \int \sigma(\vec{x}, t) dV. \quad (171)$$

The entropy production for the fluctuations around the dynamical equilibrium is given by

$$P \equiv \frac{dS}{dt} = \int \sum_{j=1}^n X_j J_j dV, \quad (172)$$

where X_i stand for the generalized forces and $J_i \equiv \dot{\alpha}_i$ the corresponding currents. We now have to impose that

$$P > 0. \quad (173)$$

Differentiating Eq.(171) with respect to time, we have

$$\frac{dP}{dt} \equiv \int \sum_{j=1}^n (\dot{X}_j J_j + X_j \dot{J}_j) dV = \frac{d_X P}{dt} + \frac{d_J P}{dt}. \quad (174)$$

Here in general we can prove[11, 12]

$$\frac{d_X P}{dt} \leq 0, \quad (175)$$

while it is not necessary that we have

$$\frac{d_J P}{dt} \leq 0. \quad (176)$$

In the linear region, we can assume that the linear relations:

$$J_i = \sum_{j=1}^n L_{ij} X_j, \quad X_i = \sum_{j=1}^n R_{ij} J_j, \quad (177)$$

hold true, where the Onsager's reciprocal relations are also assumed:

$$L_{ij} = L_{ji}, \quad R_{ij} = R_{ji}. \quad (178)$$

In this regime, we can prove that

$$\frac{d_J P}{dt} = 2 \int \sum_{i,j=1}^n (L_{ij} X_j \dot{X}_i) dV = \frac{d_X P}{dt} \leq 0. \quad (179)$$

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

$$\frac{dP}{dt} \leq 0. \quad (180)$$

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

This approach is the essence of the Prigogine's method[8–12]. Therefore, it is nothing more than the Lyapunov method in the linear stability analysis in mathematics. In this way, we can understand that the Prigogine's method in the stability of

the dynamical nonlinear systems is a natural generalization of the Onsager's method in the theory of thermal fluctuations.

What is important here is that Onsager's equation of Eq.(161) for the thermal equilibrium state holds true in the dynamical equilibrium state as well. And the meaning of Eq.(180) is the minimum principle. As long as the system lies near the dynamical equilibrium, *the entropy production must be minimum*, since we now have $P > 0, \dot{P} \leq 0$. Thus, Prigogine arrived at the concept of the *principle of the least production of entropy* for the dynamical equilibrium, generalizing the Onsager's concept of the *principle of the least dissipation of energy* for the thermal equilibrium.

There is weakness here, however. That is to say, we have always assumed that the external vector $\vec{\lambda}$ is constant from the beginning of the theory such that the dynamical equilibrium state depends upon $\vec{\lambda}$ such as $\vec{x}_{eq} = \vec{x}_{eq}(\vec{\lambda})$. As we know in chemical reactions, such external parameters λ_i ($i = \dots, r$) are the inputs and the outputs parameters such as molecules before and after chemical reactions, so that the system reacts ingredients to obtain products from the input materials. The more the input materials the more the output materials. In this sense, the external variables can control chemical reactions of the system. Thus, we are led to the concept of the *control variables* to the chemical reactions. This may be embedded in the theory of optimal control[3, 4] introduced before. This is why we are interested in such a theory.

E. The Principle of the Optimal Production of Entropy

Denote by $\vec{x} = (x_1, \dots, x_n)$ the state vector and by $\vec{u} = (u_1, \dots, u_r)$ the control vector. Let us denote by $S(\vec{x}, \vec{u}, t)$ and the entropy production by

$$P(\vec{x}, \vec{u}, t) \equiv \frac{dS(\vec{x}, \vec{u}, t)}{dt}. \quad (181)$$

Let us denote the dissipation function of energy by $\Phi(\vec{x}, \vec{u}, t)$. Let us denote \mathcal{J} by the following entropy production:

$$\begin{aligned} \mathcal{J} &\equiv \int_{t_0}^{t_1} \mathcal{L}(\vec{x}(t), \vec{u}(t), t) dt, \\ &= \int_{t_0}^{t_1} [P(\vec{x}, \vec{u}, t) - 2\Phi(\vec{x}, \vec{u}, t)] dt \\ &= \int_{t_0}^{t_1} \left[\frac{dS(\vec{x}, \vec{u}, t)}{dt} - 2\Phi(\vec{x}, \vec{u}, t) \right] dt. \end{aligned} \quad (182)$$

Here $2\Phi(\vec{x}, \vec{u}, t)$ stands for both of the Onsager's terms such as $2\Phi(\vec{\alpha}) + 2\Psi(\vec{X})$. But we do not specify the explicit expressions for them nor need do so in this paper.

Then, we seek for the condition that the functional \mathcal{J} becomes minimum under the time development of the system:

$$\dot{\vec{x}}(t) = \vec{f}(\vec{x}, \vec{u}, t). \quad (183)$$

Obviously, this idea is a natural extension of that of Onsager and Prigogine.

As was fully discussed by Onsager a long time ago, we can invoke the following condition:

$$\delta\mathcal{J} \geq 0, \quad (184)$$

$$\max_{\vec{u}} \mathcal{J} \equiv \max_{\vec{u}} \int_{t_0}^{t_1} \mathcal{L}(\vec{x}(t), \vec{u}(t), t) dt. \quad (185)$$

Now, we apply the maximum principle to the functional such that

$$\delta\mathcal{J} = 0. \quad (186)$$

As was described in §.II, we have the Pontryagin's Hamiltonian:

$$\mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}, t) \equiv \sum_{i=1}^n \psi_i(t) f_i(\vec{x}(t), \vec{u}(t), t) + \psi_0 \mathcal{L}(\vec{x}(t), \vec{u}(t), t). \quad (187)$$

Here the variable ψ_0 in front of the second term is taken so that the \mathcal{J} functional must be maximum or minimum; it depends upon the situation of the problem. Usually, $\psi_0 = 1(-1)$ is taken for the maximum(minimum) principle adjusting with the maximality(minimality) of the functional \mathcal{J} . We can take $\psi_0 = 1$ for our case here. For example, when we take \mathcal{L} as the Onsager-Prigogine's functional above, then we can regard $\psi_i(t)$ as the chemical potential divided by the temperature, $\mu_i(t)/T$, T being a constant temperature. This is essentially the correspondent of Eq.(27) and Eq.(146).

The Pontryagin's Hamiltonian satisfies the Pontryagin's Hamilton equations of motion:

$$\dot{\psi}_i = -\frac{\partial \mathcal{H}}{\partial x_i} = -\sum_{j=1}^n \psi_j \frac{\partial f_j}{\partial x_i}, \quad i = 1, \dots, n \quad (188)$$

with the optimality condition:

$$\frac{\partial \mathcal{H}}{\partial u_s} = 0, \quad s = 1, \dots, r, \quad (189)$$

and the maximum condition[7]:

$$\frac{\partial^2 \mathcal{H}}{\partial u_s^2} \leq 0, \quad s = 1, \dots, r. \quad (190)$$

This realizes the maximum (or minimum) principle of Pontryagin:

$$\mathcal{H} \leq \mathcal{M} \equiv \max_{\vec{u} \in U} \mathcal{H} = 0. \quad (191)$$

Solving Eq.(189) for the control vector $\vec{u}(t)$, analogous to the way that Prigogine solved for the dynamical equilibrium $\vec{x}(t) = \vec{x}_{eq}(\vec{\lambda}) = \text{const.}$, we obtain the control vector $\vec{u}(t)$ as a function of $\vec{\psi}$ and \vec{x} such that

$$\vec{u}(t) = \vec{u}_{opt}(\vec{\psi}, \vec{x}). \quad (192)$$

Substituting this into the Pontryagin's Hamiltonian \mathcal{H} , we obtain

$$\mathcal{H}_{opt} \equiv \mathcal{H}(\vec{\psi}, \vec{x}, \vec{u}_{opt}(\vec{\psi}, \vec{x}), t). \quad (193)$$

Using this for Eq.(188), we finally obtain the following Hamilton equations of motion:

$$\dot{\psi}_i = -\frac{\partial \mathcal{H}_{opt}}{\partial x_i}, \quad (194)$$

$$\dot{x}_i = \frac{\partial \mathcal{H}_{opt}}{\partial \psi_i}, \quad (195)$$

which by definition provides the optimal motion of the system.

In order to know the explicit expression of the optimality condition, let us substitute Eq.(187) into Eq.(189). Then, we are led to the following:

$$\begin{aligned} \frac{\partial \mathcal{H}}{\partial u_s} &= \sum_{i=1}^n \psi_i(t) \frac{\partial f_i(\vec{x}(t), \vec{u}(t), t)}{\partial u_s} + \frac{\partial \mathcal{L}(\vec{x}(t), \vec{u}(t), t)}{\partial u_s} \\ &= \sum_{i=1}^n \psi_i(t) \frac{\partial f_i(\vec{x}(t), \vec{u}(t), t)}{\partial u_s} + \frac{\partial [\dot{S}(\vec{x}, \vec{u}, t) - 2\Phi(\vec{x}(t), \vec{u}(t), t)]}{\partial u_s} = 0, \end{aligned} \quad (196)$$

for $s = 1, \dots, r$. From this, obviously, if there is no control parameters in the equations of motion $\dot{x}_i = f_i(\vec{x}(t), \vec{u}(t), t) = f_i(\vec{x}(t), t)$, then the first term vanishes. Then, we obtain the principle of the optimal production of the entropy as

$$\frac{\partial [\dot{S}(\vec{x}, \vec{u}, t) - 2\Phi(\vec{x}, \vec{u}, t)]}{\partial u_s} = 0, \quad (197)$$

for $s = 1, \dots, r$. This is obviously the natural generalization of the Onsager-Prigogine's theory. Thus, our claim has been proved.

This is the essence of the concept of the optimal production of entropy as well as the concept of the optimal dissipation of energy.

Let us note the physical meaning of the maximum principle. As was shown before, if we use suitable choice for the Pontryagin's vector $\vec{\psi}$, then we can define the units of the Hamiltonian so as to become the power of the system such as

$$\mathcal{H} = \mathcal{W} = \frac{dE}{dt}. \quad (198)$$

Seeing Eq.(191), the maximum value \mathcal{M} of the Hamiltonian \mathcal{H} is zero; namely,

$$\mathcal{W} = \frac{dE}{dt} = 0. \quad (199)$$

Hence, when the system realizes the maximum of the Hamiltonian, then the power of the system approaches zero; it means *the energy is conserved* at this moment! Thus, the energy conservation law is recovered!

This means that when the system approaches the most effective state under the optimal control, the system have to obey the energy conservation law. However, in this case of an open system unlike a closed system, the input and the output exist such that the former pours energy into the system from the outside and the latter dissipates energy to the outside of the system, both of which can change in time. There is always an energy flow from the outside into the inside and from the inside into the outside, which are controlled by the control vector of the system. Nevertheless, the total energy is conserved. This seems to be the physical meaning of the maximum principle of Pontryagin described in terms of the language of physicists.

In this way, even though we start with an open system described by the system of nonlinear differential equations with the control parameters as input and output for the system [see Eq.(3)], the maximum principle assures that the system realizes the energy conservation so that the power vanishes when the system approaches the optimal state.

V. CONCLUSION

In conclusion, we have presented the physical foundation for the Pontryagin's maximum principle[3, 4, 7] from the various aspects. First, in §.II we introduced the Euler-Lagrange's method for deriving the maximum principle[5]. Second, in §.III we introduced the variational method for deriving the maximum principle[6]. Third, in §.IV we discussed the theory of the non-equilibrium thermodynamics in the optimal control processes, which is new. This section is most important in physics.

Especially, we have first discussed the Rayleigh's theory of the dissipative system in classical mechanics, where the principle of the least dissipation of energy is highlighted. Second, we have discussed the Onsager's theory of the irreversible processes in equilibrium thermodynamics, where the principle of the least dissipation of free energy is highlighted. And third we have discussed the Prigogine's theory of the dissipative structure in dynamical systems, where the principle of the least production of entropy is highlighted. respectively.

And finally, by considering the Onsager-Prigogine's energy dissipation and entropy production function as the Lagrangian in the meaning of Pontryagin, and by applying the above modern optimal control theory, we have obtained the concept of the principle of the optimal dissipation of energy as well as the concept of the principle of the optimal production of entropy in the optimal control systems.

And hence, we have shown that even though we start with an open system described by the system of nonlinear differential equations with the control parameters as input and output for the system [see Eq.(3)], the Pontryagin's maximum principle assures that the system realizes the energy conservation so that the power vanishes when the system approaches the optimal state. This is the main result of the present paper.

Appendix A: Theoretical Framework of Classical Mechanics

1. 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:

$$\frac{d\vec{x}}{dt} = \frac{\partial H}{\partial \vec{p}}, \quad \frac{d\vec{p}}{dt} = -\frac{\partial H}{\partial \vec{x}}. \quad (\text{A1})$$

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

$$\frac{d\vec{x}}{dt} = \frac{\vec{p}}{m} = \vec{v}, \quad \frac{d\vec{p}}{dt} = -\frac{\partial V(\vec{x})}{\partial \vec{x}}. \quad (\text{A2})$$

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

$$\frac{dH}{dt} = \frac{\partial H}{\partial \vec{x}} \cdot \frac{d\vec{x}}{dt} + \frac{\partial H}{\partial \vec{p}} \cdot \frac{d\vec{p}}{dt} = \frac{\partial H}{\partial \vec{x}} \cdot \frac{\partial H}{\partial \vec{p}} - \frac{\partial H}{\partial \vec{p}} \cdot \frac{\partial H}{\partial \vec{x}} = 0, \quad (\text{A3})$$

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

2. 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

$$S = \int_{t_0}^{t_1} L dt = \int_{t_0}^{t_1} L(\vec{x}, \dot{\vec{x}}) dt. \quad (\text{A4})$$

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

$$\delta S = 0. \quad (\text{A5})$$

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

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\vec{x}}} \right) - \frac{\partial L}{\partial \vec{x}} = 0. \quad (\text{A6})$$

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 stand 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*.

3. 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

$$S(t) = \int_{t_0}^t L dt = \int_{t_0}^t L(\vec{x}, \dot{\vec{x}}) dt. \quad (A7)$$

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 Euler-Lagrange equation of Eq.(19). Taking the time variation δS , we find

$$\delta S = \left[\frac{\partial L}{\partial \dot{\vec{x}}} \cdot \delta \vec{x} \right]_{t_1}^t + \int_{t_1}^t \left(\frac{\partial L}{\partial \vec{x}} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\vec{x}}} \right) \cdot \delta \vec{x} dt. \quad (A8)$$

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

$$\delta S = \frac{\partial L}{\partial \dot{\vec{x}}} \cdot \delta \vec{x}(t) = \vec{p} \cdot \delta \vec{x}(t), \quad (A9)$$

where we have defined as

$$\vec{p} = \frac{\partial L}{\partial \dot{\vec{x}}}. \quad (A10)$$

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

$$\frac{dS}{dt} = L. \quad (A11)$$

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

$$\frac{dS}{dt} = \frac{\partial S}{\partial t} + \frac{\partial S}{\partial \vec{x}} \cdot \dot{\vec{x}} = \frac{\partial S}{\partial t} + \vec{p} \cdot \dot{\vec{x}} = L. \quad (A12)$$

Let us define the Hamiltonian H as

$$H = \vec{p} \cdot \dot{\vec{x}} - L. \quad (A13)$$

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

$$\frac{\partial S}{\partial t} + H = 0. \quad (A14)$$

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

$$\vec{p} \equiv \frac{\partial S}{\partial \vec{x}}. \quad (A15)$$

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

$$\frac{\partial S(\vec{x}, t)}{\partial t} + H\left(\vec{x}, \frac{\partial S}{\partial \vec{x}}\right) = 0. \quad (A16)$$

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 reach the final point. Instead, this needs at any instant the orbit have 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 .

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