Thermodynamic Irreversibility from high-dimensional Hamiltonian Chaos

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(Received November 9, 1999)

This paper discusses the thermodynamic irreversibility realized in high-dimensional Hamiltonian systems with a time-dependent parameter. A new quantity, the irreversible information loss, is defined from the Lyapunov analysis so as to characterize the thermodynamic irreversibility. It is proved that this new quantity satisfies an inequality associated with the second law of thermodynamics. Based on the assumption that these systems possess the mixing property and certain large deviation properties in the thermodynamic limit, it is argued reasonably that the most probable value of the irreversible information loss is equal to the change of the Boltzmann entropy in statistical mechanics, and that it is always a non-negative value. The consistency of our argument is confirmed by numerical experiments with the aid of the definition of a quantity we refer to as the excess information loss.

§1. Introduction

Thermodynamics formalizes a fundamental limitation of possible processes between equilibrium states. In particular, when a thermodynamic system is enclosed by adiabatic walls, the limitation is represented by, for example, a fact that, given a system in some initial state, it is not possible to lower the system’s energy by first changing some of its other extensive variables and then returning them to their original values. Contrastingly, the energy of the system can be increased by the similar change of the other extensive variables. These two facts make clear the special nature of energy as an extensive variable. This asymmetry is the basis of thermodynamic irreversibility.

Thermodynamics is one of the most elegant theories being based on only a few fundamental principles. However, one may wonder how its principles emerge out of purely mechanical systems. Thermodynamic systems consist of many molecules, whose dynamics are described by Hamiltonian equations. Thus, in the idealized limit of adiabatic walls, a thermodynamic system can be regarded as a Hamiltonian system that is connected to some mechanical apparatus, but does not contact a heat reservoir. With this in mind, it may be natural to expect that thermodynamic irreversibility can be formalized in Hamiltonian systems.

Thermodynamic entropy plays a central role in the description of thermodynamic irreversibility, and the thermodynamic entropy is generally thought to be given by the logarithm of the number of micro-states. This relation, the Boltzmann formula, seems well-established as far as the calculation of equilibrium values is concerned. However, it has not yet been shown that the Boltzmann formula provides a complete account of irreversibility.

In this paper, we discuss thermodynamic irreversibility based on the nature of high-dimensional Hamiltonian chaos. As our most notable result, we find a new quantity which satisfies an inequality associated with thermodynamic irreversibility. We define this quantity, the “irreversible information loss”, from dynamical system considerations. Furthermore, we argue reasonably that the irreversible information loss is related to the change of the Boltzmann entropy, and this leads us to conclude that the Boltzmann entropy does not decrease for any processes in the thermodynamic limit.

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1.1. Related studies

This paper provides theoretical arguments for numerical results reported in a previously published paper, and contains a detailed description of the numerical experiment.

The present study has been carried out under the influence of several related studies. First, the attempt to construct steady state thermodynamics by Oono and Paniconi has provided the direction of the present study. They have proposed an operational method to obtain non-equilibrium thermodynamic functions. In addition, from a more general viewpoint, they emphasize the importance of theory concerning the relation between two different states. Following this manner of thinking, we have set out to study thermodynamic irreversibility from dynamical systems.

The stochastic energetics proposed by Sekimoto has given a nice example of the construction of thermodynamics from dynamical systems. Stochastic energetics formalizes energy transformation in Langevin dynamics with a clear distinction between heat and work. Sekimoto and Sasa have demonstrated the minimum work principle and defined the free energy from this principle. Their argument also includes a complementary relation which defines a new thermodynamic function of two state variables. Recently, Sekimoto and Oono have constructed an example of steady state thermodynamics by analyzing a Langevin dynamical model.

The minimum work principle can be formulated through an equality proposed by Jarzinski. This equality may provide a method to find inequalities related to thermodynamics. In fact, Hatano has proved a Jarzinski-type equality for the transition between steady states under a certain condition and has derived an inequality related to the steady state thermodynamics.

As discussed by Crooks, the Jarzinski’s equality is also related to the fluctuation theorem proposed by Evans, Cohen and Morriss. The fluctuation theorem claims a peculiar property of the probability of the finite time average of the entropy production in a non-equilibrium steady state. Gallovotti and Cohen have presented a mathematical proof of the fluctuation theorem based on the assumption that the steady state measure is given by the dynamical measure. Since that time, it has been shown that the fluctuation theorem holds even in stochastic systems. On general grounds, Maes has presented an argument that the fluctuation theorem can be understood by a Gibbs property of the space-time measure.

Transportation coefficients in non-equilibrium steady states have been expressed in terms of dynamical system quantities. There are two different approaches for this. In one approach, the viscosity is related to the sum of all Lyapunov exponents in a Hamiltonian system supplemented with a deterministic thermostating force. The other approach applies to Hamiltonian systems with open boundary conditions. Here, the diffusion constant is related to the escape rate which is obtained in terms of the difference between the sum of the positive Lyapunov exponents and the Kolmogorov-Sinai entropy.

Finally, we mention some recent developments in the understanding of thermodynamics. Lieb and Yngvason wrote an important paper on axiomatic thermodynamics. They have given an explicit expression of the thermodynamic entropy based on a set axioms concerning the adiabatic accessibility, and have proven the entropy principle, the second law of thermodynamics. Although their formulation is fully mathematical, the idea of the explicit expression of thermodynamic entropy can be translated into standard energetic thermodynamics.

1.2. Outline of the paper

This paper consists of nine sections, each of which consists of several subsections. In order to give a self-contained explanation, we include a review of thermodynamics, Hamiltonian systems, Boltzmann entropy, and Lyapunov analysis. Some of these are no doubt rather well-known topics to specialists. However, there are not a large number of people who understand all of them well. Also, it was our intention to write this paper so that it can be understood by non-specialists, who have interest in the relation between thermodynamic irreversibility and dynamical systems. The organization of the paper is summarized below.

In Section 2 we start with a review of thermodynamics in an adiabatic environment. Ther-
dynamic irreversibility is precisely defined based on basic notions such as state and process. The essence of the thermodynamic entropy is described by the entropy principle. We then explain the reason why a Hamiltonian system with a time-dependent parameter provides a model for a thermodynamic system in an adiabatic environment. We assume the microcanonical measure for the initial conditions and that the systems possess the mixing property with respect to the measure. We also assume the existence of certain large deviation properties in order to establish correspondence with the extensivity of thermodynamics. Based on these assumptions, we define the equilibrium state and most probable process in Hamiltonian systems. After these preliminaries, we address a main question.

In Section 3 we first review the Boltzmann formula in statistical mechanics. In particular, defining the time-dependent Boltzmann entropy, we derive a simple form of the Boltzmann entropy change for general processes. Using this formula, we calculate the average of the Boltzmann entropy change for a step process, where the average is taken over the initial conditions sampled from the microcanonical ensemble on an energy surface. We show that the average value is positive in the thermodynamic limit. We further find that the average value is related to the fluctuation of the Boltzmann entropy change.

In Section 4 we review the Lyapunov analysis, which is a standard method to study chaotic dynamical systems with numerical experiments. We start with the Gram-Schmidt decomposition, because it is the easiest computational technique for the Lyapunov analysis. We then discuss the convergence property of an orthogonal frame. Since the orthogonal frame obtained from convergence does not satisfy the transitive property, we define Lyapunov vectors from the orthogonal frame so that this property is satisfied. Based on these Lyapunov vectors, we define Lyapunov exponents, local expansion ratios, and the information loss rate. In order to recover the symmetry of unstable and stable directions, we also define contraction ratios. We then prove a relation between the expansion and contraction ratios. We also derive an expression for the weight on trajectory segments.

In Section 5 we discuss the reversibility of Hamiltonian systems. We relate the evolution map, Lyapunov vectors, and local expansion rates for time-reversed systems to those for the original system. The reversibility leads to a reversibility paradox. In order to resolve the paradox, we need to consider the measure for a set of the initial conditions for time-reversed systems. This consideration leads to a reversibility relation expressed in terms of probability.

In Section 6 we begin with the definition of irreversible information loss. Using the reversibility relation mentioned above, we prove that the irreversible information loss averaged over the initial conditions is always non-negative. We define the most probable value of the irreversible information loss in the thermodynamic limit, and we present an argument that this most probable value is equal to the Boltzmann entropy change.

In Section 7 we define a quantity we call excess information loss, because this quantity is more tractable than the irreversible information loss. We present a relation between the Boltzmann entropy change and the excess information loss based on the assumption that the reversible part of the excess information loss is equal to the quasi-static excess information loss. This relation is identical to an equality proposed in a previous paper. Furthermore, we briefly discuss a minimum excess information loss principle, which may be analogous in some sense to the minimum work principle in thermodynamics with an isothermal environment. We also explain the origin of the quasi-static excess information loss using Lyapunov analysis.

In Section 8 we report results of numerical experiments on a Fermi-Pasta-Ulam model with a time-dependent nonlinear term. With these, we numerically check the assumptions in the arguments given in the previous sections, and numerically demonstrate several properties of certain quantities such as the Lyapunov exponents and Boltzmann entropy changes in this model. As the main numerical experiment, we confirm the relation between the Boltzmann entropy change and the excess information loss.

The final section is devoted to concluding remark.
1.3. Remarks

Our theoretical arguments include some non-rigorous, but intuitively reasonable statements. To as great an extent as possible, we state explicitly when the assertions we make are assumptions. There is one exception, however. We often use the expression $o(N)$ to represent a quantity of negligible magnitude compared to $N$ in the limit $N \to \infty$. This constitutes an order estimate valid in the case that the system satisfies an appropriate condition. However, we do not discuss what this condition is, nor do we explicitly state that an assumption is involved when we neglect such a quantity. We simply expect that the condition is satisfied unless an abnormal situation occurs.

We use the same font for numbers and vectors. We believe that the difference can be understood in the context. Also, a matrix is expressed as $A$, and $A_{ij}$ denotes the $(ij)$-element of this matrix.

§2. Preliminary

In this section, we review thermodynamics and Hamiltonian systems. We clarify basic assumptions of our theory and address the main question of this paper.

2.1. Thermodynamic irreversibility

A thermodynamic system is characterized by the internal energy $U$ and a set of work variables $\{X_i\}$. When the value of $X_i$ is changed externally, the energy change is induced. The infinitely small response $dU$ is written as

$$dU = \sum_i Y_i dX_i. \quad (2.1)$$

In thermodynamics, $X_i$ is chosen as an extensive or intensive variable. Since the internal energy $U$ is an extensive variable, $Y_i$ is an intensive or extensive variable, respectively. The relation Eq. (2.1) is valid for the case that the system is enclosed by adiabatic walls. More formally, Eq. (2.1) should be regarded as a mathematical expression of a physical situation that the system is placed in an adiabatic environment.

The equilibrium state $\Sigma$ is assumed to be realized when the system is left for a sufficiently long time after values of the work variables are fixed. This assumption provides the operational definition of the equilibrium state. Also, the equilibrium state $\Sigma$ is assumed to be determined uniquely by a set of the values of $(U, \{X_i\})$. That is, the state $\Sigma$ is identified with $(U, \{X_i\})$. When the value of $X_i$ is changed externally, a transition from an equilibrium state $\Sigma_0$ to another one $\Sigma_1$ occurs. This transition, which is denoted by $\Sigma_0 \xrightarrow{a} \Sigma_1$, is called the thermodynamic process or simply the process. More precisely, the process is called the adiabatic process realized in an adiabatic environment. However, in the argument below, we use the term process instead of adiabatic process.

Let $\Sigma_0$ and $\Sigma_1$ be arbitrary equilibrium states. We then ask whether or not processes $\Sigma_0 \xrightarrow{a} \Sigma_1$ and $\Sigma_1 \xrightarrow{a} \Sigma_0$ are realizable. When both the processes are realizable, these are called reversible processes. When only one process $\Sigma_0 \xrightarrow{a} \Sigma_1$ is realizable, this process is called the irreversible process. We can easily see that the process

$$(U, \{X_i\}) \xrightarrow{a} (U', \{X_i\}) \quad (2.2)$$

provides an example of irreversible processes when $U' > U$.

The essence of the thermodynamic entropy is described by the entropy principle:

There exists an extensive variable $S$ given by a function of $\Sigma$ such that the inequality

$$S(\Sigma_1) \geq S(\Sigma_0) \quad (2.3)$$

is satisfied if and only if a process $\Sigma_0 \xrightarrow{a} \Sigma_1$ is realizable. The extensive variable $S$ is determined uniquely up to multiplicative and additive arbitrary constants.

Lieb and Yngvason have proved the entropy principle based on the axioms concerning the adiabatic accessibility. Also, in conventional thermodynamics based on work and heat, the entropy principle can be proved on some physical assumptions.
2.2. Hamiltonian systems

A Hamiltonian system is characterized by a Hamiltonian function \( H(\Gamma) \), where \( \Gamma \) is a set of canonical coordinates \( \{q_i\} \) and momentums \( \{p_i\} \)

\[
\begin{align*}
\Gamma_i &= q_i, \\
\Gamma_{N+i} &= p_i,
\end{align*}
\]

(2.4)

(2.5)

where \( 1 \leq i \leq N \). Equations of motion for \( q_i \) and \( p_i \) are given by

\[
\begin{align*}
\frac{dq_i}{dt} &= \frac{\partial H}{\partial p_i}, \\
\frac{dp_i}{dt} &= -\frac{\partial H}{\partial q_i}.
\end{align*}
\]

(2.6)

(2.7)

These equations are formally written as

\[
\frac{d\Gamma}{dt} = -J \frac{\partial H}{\partial \Gamma},
\]

(2.8)

where \( J \) is a \( 2N \times 2N \) anti-symmetric matrix which satisfies

\[
J^2 = -1.
\]

(2.9)

Under an initial condition \( \Gamma(0) \) given at \( t = 0 \), the phase space point at time \( t \), \( \Gamma(t) \), is determined by the equation of motion.

In this paper, we are concerned with Hamiltonian systems with a time-dependent parameter \( \alpha \). The energy of the system \( E \) at time \( t \) is given by

\[
E(t) = H(\Gamma(t), \alpha(t)).
\]

(2.10)

We then obtain the equality

\[
\frac{dE}{dt} = \sum_{i=1}^{N} \left( \frac{\partial H}{\partial q_i} \frac{dq_i}{dt} + \frac{\partial H}{\partial p_i} \frac{dp_i}{dt} \right) + \frac{\partial H}{\partial \alpha} \frac{d\alpha}{dt},
\]

(2.11)

(2.12)

where we have used the equations of motion. This equality is rewritten as

\[
\frac{dE}{dt} = Ad\alpha,
\]

(2.13)

where

\[
A = \frac{\partial H}{\partial \alpha}.
\]

(2.14)

Comparing Eq. (2.13) with Eq. (2.1), we find that \( E \) and \( \alpha \) correspond to the internal energy \( U \) and a work variable \( X \). This suggests that a Hamiltonian system with a time-depending parameter can be a dynamical system model for thermodynamics in an adiabatic environment. We proceed to our discussion based on this expectation and attempt to find necessary issues so as to establish consistency with thermodynamics.

Since we are particularly interested in thermodynamic processes, we assume that the value of \( \alpha \) is changed in a finite time interval \( [\tau_i, \tau_f] \), that is,

\[
\frac{d\alpha(t)}{dt} = 0
\]

(2.15)

when \( t \not\in [\tau_i, \tau_f] \). In the argument below, we assume the condition

\[
0 \ll \tau_i \leq \tau_f
\]

(2.16)

without an explicit remark. Note that \( \ll \) in Eq. (2.16) has been assumed for a technical reason. We also represent the protocol of the parameter change by \( \alpha() \).
2.3. Measure

We assume that the initial condition given at \( t = 0 \) is sampled from the microcanonical ensemble on an energy surface \( \Sigma \). The measure for the ensemble is given by the microcanonical measure

\[
\mu_{mc}(d\Gamma; \Sigma) = \frac{1}{|\Sigma|} \frac{1}{|\nabla \Gamma H|} d\sigma,
\]

where \( d\sigma \) is the Lebesgue measure on the energy surface, and \(|\Sigma|\) is given by

\[
|\Sigma| = \int d\sigma \frac{1}{|\nabla \Gamma H|}.
\]

\( \mu_{mc}(\Gamma; \Sigma) \) and \(|\Sigma|\) are rewritten as

\[
\mu_{mc}(d\Gamma; \Sigma) = \frac{1}{|\Sigma|}d\Gamma \delta(H(\Gamma) - E),
\]

\[
|\Sigma| = \int d\Gamma \delta(H(\Gamma) - E),
\]

where \( d\Gamma \) is the 2\( N \)-dimensional Lebesgue volume element in the phase space. We also notice that Eq. (2.19) is given by

\[
\mu_{mc}(\Delta_{\epsilon}(\Gamma); \Sigma) = \lim_{\delta E \to 0} \frac{\mu_L(\Delta_{\epsilon}(\Gamma) \cap \Sigma \circ \delta E)}{\mu_L(\Sigma \circ \delta E)}
\]

where \( \Sigma \circ \delta E \) denotes a union of energy surfaces from \( E \) to \( E + \delta E \), \( \Delta_{\epsilon}(\Gamma) \) is a region with a size \( \epsilon \) which includes a point \( \Gamma \), and \( \mu_L \) is the 2\( N \) dimensional Lebesgue measure.

We also assume that the systems in question possess are ergodic and process the mixing property. Here, a system is called ergodic with respect to the microcanonical measure, when the equality

\[
\lim_{T \to \infty} \frac{1}{T} \int_0^T dt f(\Gamma(t)) = \int \mu_{mc}(d\Gamma; \Sigma) f(\Gamma)
\]

holds for an arbitrary measurable function \( f \) and almost all initial conditions \( \Gamma(0) \) with respect to the measure. The mixing property with respect to the microcanonical measure means that the equality

\[
\lim_{t \to \infty} \int \mu_{mc}(d\Gamma(0); \Sigma) f(\Gamma(0)) g(\Gamma(t)) = \int \mu_{mc}(d\Gamma; \Sigma) f(\Gamma) \int \mu_{mc}(d\Gamma; \Sigma) g(\Gamma)
\]

holds for arbitrary measurable functions \( f \) and \( g \). It is easily proved that a mixing system possesses the ergodicity.

Suppose that the initial condition at time \( t = -t', t' > 0 \), is sampled from an ensemble with the measure

\[
\mu_f(d\Gamma(-t'); \Sigma) = \mu_{mc}(d\Gamma(-t'); \Sigma) f(\Gamma(-t'))
\]

where \( f \) is a measurable function normalized in such a way that

\[
\int_{\Sigma} \mu_{mc}(d\Gamma(-t'); \Sigma) f(\Gamma(-t')) = 1.
\]

Then, the mixing property leads to

\[
\lim_{t' \to \infty} \int \mu_f(d\Gamma(-t'); \Sigma) g(\Gamma(0)) = \int \mu_{mc}(d\Gamma; \Sigma) g(\Gamma).
\]

That is, the average of \( g(\Gamma(0)) \) with respect to \( \mu_f(d\Gamma(-t'); \Sigma) \) is the same as the average of \( g(\Gamma(0)) \) with respect to \( \mu_{mc}(d\Gamma(0); \Sigma) \) when \( t' \to \infty \). Using Eq. (2.26), we check numerically the validity of the mixing property and we can prepare the microcanonical ensemble at \( t = 0 \) in the following way.

First, we prepare a set of the initial conditions at \( t = -t' \) sampled from an ensemble with a measure absolutely continuous with respect to the Lebesgue measure on the energy surface \( \Sigma \). (It
can be done easily in numerical experiments.) Then, we take an average of a dynamical variable, for example \( A \), at \( t = 0 \). We carry out two experiments for two different measures assumed at \( t = -t' \). If the average values coincide, we may regard that the system possesses the mixing property.

Also, from Eq. (2.26), we find that this average value is the average for the microcanonical measure at \( t = 0, \mu_{mc}(d\Gamma; \Sigma) \). This implies that we can prepare the microcanonical ensemble at \( t = 0 \).

### 2.4 Thermodynamic limit

In thermodynamics, the internal energy \( U \) is an extensive variable, and a work variable is an extensive or intensive variable. In order to establish the consistency with thermodynamics, we assume the following large deviation property [22] which may be closely related to the extensivity of the energy:

Let \( \Pi_E(E_1)dE \) be a probability that final energy after the parameter change takes a value in the region \([E_1, E_1 + dE]\). Then, \( \Pi_E \) is written in the form

\[
\Pi_E(E_1) \sim \exp(-N\phi_E(E_1/N)),
\]

(2.27)

in the appropriate asymptotic limit including \( N \to \infty \).

Several remarks are mentioned. (i) The appropriate limit in Eq. (2.27) is called the thermodynamic limit. In the argument below, the limit \( N \to \infty \) always implies the thermodynamic limit without an explicit remark. (ii) The probability of final energy is induced from the measure for the ensemble of the initial conditions. (iii) \( \phi_E \) is called a rate function, and is a non-negative convex function with zero. The zero of \( \phi_E \), \( \bar{E}_{1*} \), is called the most probable value of \( E_1/N \).

We next discuss the extensivity or intensivity of \( \alpha \). We pay attention to the case that \( \alpha \) is an intensive parameter. (The reversed case is similarly discussed.) The variable \( A \) then turns out to be an extensive variable, which is characterized by the large deviation property:

Let \( \Pi_A(A')dA \) be a probability that \( A \) takes a value in the region \([A', A' + dA]\) at \( t = 0 \). Then, \( \Pi_A \) is written in the form

\[
\Pi_A(A') \sim \exp(-N\phi_A(A'/N)),
\]

(2.28)

in the thermodynamic limit.

Note that the probability density \( \Pi_A \) is determined by the measure for the ensemble. Since the most probable value of \( A/N, \bar{A}_* \), exists for each energy surface, we write \( \bar{A}_*(\Sigma) \) when we emphasize the state dependence.

### 2.5 Equilibrium state

We assume that the equilibrium state in thermodynamics corresponds uniquely to the energy surface. That is the reason why we used the same symbol \( \Sigma \) of an energy surface in Section 2.3 as the equilibrium state in Section 2.1. Also, the energy surface is specified by a set of quantities \((E, \alpha)\). In the argument below, \( \Sigma \) denotes an equilibrium state, an energy surface and a set of quantities \((E, \alpha)\).

Let us discuss a condition under which we can know whether or not the equilibrium state is realized. The term ‘equilibrium’ implies that nothing changes due to the balance. Thus, it is natural to find a quantity which does not change at equilibrium. Although the energy \( E \) does not change when \( t \geq \tau_f \), it is strange that the equilibrium state is realized immediately after the parameter change is finished. The energy cannot be used as an indicator of the equilibrium state. The next candidate of the indicator may be the variable \( A \). However, since the trajectory never converges to a fixed point, the value of \( A \) remains time-dependent. We then notice here that the argument for the nature of equilibrium should be developed with the thermodynamic limit.

Suppose that \( \Gamma(\tau_f) \in \Sigma_1 \). In general, \( A(\tau_f)/N \) is not equal to \( \bar{A}_*(\Sigma_1) \). However, from large deviation and mixing properties, we can expect

\[
\lim_{t \to \infty} \frac{A(t)}{N} \to \bar{A}_*(\Sigma_1)
\]

(2.29)

* However, precisely speaking, this is nothing but a confirmation of one of necessary conditions for the mixing property.
in the thermodynamic limit. When \( A(t)/N \) is sufficiently close to \( A_\ast(S_1) \) up to a certain time, we assume that the state is at the equilibrium. There may be other important physical quantities to be checked. However, since we do not have any criteria for the importance, we assume that the relaxation of the variable \( A \) is enough to identify the equilibrium state.

2.6. Most probable process

Suppose that an equilibrium state \( \Sigma_0 \) is realized at \( t = 0 \) and that another equilibrium state is realized in an energy surface \( \Sigma_1 \) after a sufficiently long time from \( t = \tau_f \). We call this transition a process in the similar way as thermodynamics. However, since \( \Sigma_1 \) depends on \( I(0) \), \( \Sigma_1 \) is not determined uniquely when we assume the initial energy surface \( \Sigma_0 \) and the protocol of the parameter change \( \alpha() \). Here, in order to establish the correspondence with thermodynamics, we assume that the large deviation property of the path of \( E \)

\[
\Pi_{E:\text{path}}(\{E'(t), 0 \leq t' \leq \tau\}) \prod dE(t) \text{ be a path probability that } E(t) \text{ takes a value in the region } [E', E' + dE(t)] \text{ at time } t.\text{ Then, } \Pi_{E:\text{path}} \text{ is written in the form}
\]

\[
\Pi_{E:\text{path}}(\{E'(t), 0 \leq t' \leq \tau\}) \sim \exp(-N\phi_{E:\text{path}}(\{E'(t)/N, 0 \leq t' \leq \tau\}), \quad (2.30)
\]
in the thermodynamic limit.

The probability density \( \Pi_{E:\text{path}} \) is determined by the measure for the ensemble of the initial conditions. The rate function \( \phi_{E:\text{path}} \) is a function of path segments \( \{E'(t)/N, 0 \leq t' \leq \tau\} \), and there is a most probable path \( \{\bar{E}_s(t'), 0 \leq t' \leq \tau\} \) which minimizes the rate function. Then, since the parameter is changed in a deterministic way, the most probable process is defined as \( \{(N\bar{E}_s(t'), \alpha(t')), 0 \leq t' \leq \tau_f\} \). The most probable process is denoted by

\[
\Sigma_0 \to_s \Sigma_1, \quad (2.31)
\]

where \( \Sigma_1 = (N\bar{E}_s(\tau_f), \alpha(\tau_f)) \), and it is identified with the thermodynamic process \( \Sigma_0 \to \Sigma_1 \).

2.7. Main question

Let us summarize our basic assumptions and address the main question. When one attempts to study thermodynamic irreversibility in Hamiltonian systems, there seem three problems. The first problem is related to the measure for the initial conditions, where, as one example, a condition which determines the most natural measure is concerning. The second problem is related to the reason why macroscopic variables behave in a deterministic way. The discussion of large deviation properties is one way to consider the problem.

In this paper, we do not enter these problems deeply. As mentioned above, we assume that Hamiltonian systems in question possess the mixing property with respect to the microcanonical measure, and we also assume the large deviation properties of \( A \) and \( E \) in the thermodynamic limit. Nevertheless, we believe that there is still an important problem to be solved. We ask how the thermodynamic law is established. In other word, we ask whether or not we can find a state variable satisfying the entropy principle from dynamical systems. Let us write the question explicitly.

Let \( \Sigma_0 \to_s \Sigma_1 \) be an arbitrary most probable process. Then, find a state variable \( S \) such that

\[
S(\Sigma_1) \geq S(\Sigma_0), \quad (2.32)
\]

where the equality holds only when the reversed process \( \Sigma_1 \to_s \Sigma_0 \) is realizable.

§3. Statistical mechanics

In statistical mechanics, the thermodynamic entropy is calculated as the Boltzmann entropy. We then review fundamental properties of the Boltzmann entropy and discuss whether or not we can answer to the main question by using the Boltzmann entropy.

* Formally, we should consider the limit \( N \to \infty \) before the limit \( t \to \infty \). In the experiment with finite \( N \), we should focus on an asymptotic regime up to a certain time.
The thermodynamic entropy takes a constant value along an arbitrary quasi-static process $\Sigma_0 \rightarrow \Sigma_1$, which is realized by infinitely slow change of the parameter value. Then, in developing statistical mechanics, we first attempt to find such a quantity. The adiabatic theorem ensures the existence of an invariant quantity along quasi-static processes. We thus start with the adiabatic theorem.

3.1. Adiabatic theorem

Let $\Omega(\Sigma)$ be the phase space volume enclosed by an energy surface $\Sigma = (E, \alpha)$.

$$\Omega(E, \alpha) = \int d\Gamma \delta(E - H(\Gamma, \alpha)).$$

When the value of $\alpha$ is changed in time, the energy of the system changes. We define the time evolution of the phase space volume as

$$\Omega(t) = \Omega(E(t), \alpha(t)),$$

where note that $E(t)$ depends on $\Gamma(0)$. We then obtain

$$\frac{d\Omega}{dt} = \left[ \frac{\partial \Omega}{\partial \alpha} + \frac{\partial \Omega}{\partial E} A \right] \frac{d\alpha}{dt},$$

where we have used the equality

$$\frac{dE}{dt} = A \frac{d\alpha}{dt},$$

which is given by Eq. (2.12).

By using the expression Eq. (3.1), we derive

$$\frac{\partial \Omega}{\partial E} = |\Sigma|,$$

$$\frac{\partial \Omega}{\partial \alpha} = -|\Sigma| \langle A \rangle_\Sigma,$$

where $|\Sigma|$ and $\langle f \rangle_\Sigma$ are defined as

$$|\Sigma| = \int d\Gamma \delta(E - H(\Gamma, \alpha)),$$

$$\langle f \rangle_\Sigma = \frac{1}{|\Sigma|} \int_\Sigma \frac{d\sigma}{|\nabla \Gamma H|} f(\Gamma).$$

$\langle f \rangle_\Sigma$ corresponds to the average of $f$ over the micro-canonical ensemble on the energy surface $\Sigma$. Substituting Eqs. (3.5) and (3.6) into Eq. (3.3), we obtain

$$\frac{d\Omega}{dt} = |\Sigma| (A - \langle A \rangle_\Sigma) \frac{d\alpha}{dt},$$

where we have defined a new variable $\delta A$ as

$$\delta A = A - \langle A \rangle_\Sigma.$$

We now prove the adiabatic theorem which states that the equality

$$\Omega(\Sigma_0) = \Omega(\Sigma_1)$$

holds for an arbitrary quasi-static process $\Sigma_0 \rightarrow \Sigma_1$.

(proof)
Put $\Sigma_0 = (E_0, \alpha_0)$ and $\Sigma_1 = (E_\infty, \alpha_\infty)$. We decompose the quasi-static process into $n$ quasi-static processes such that

$$\alpha_j, E_j \xrightarrow{qs} \alpha_{j+1}, E_{j+1},$$

where $0 \leq j \leq n-1$, and $\alpha_{j+1} = \alpha_j + \Delta \alpha$ with

$$\Delta \alpha = \frac{\alpha_\infty - \alpha_0}{n}.$$  

Note that $\alpha_n = \alpha_\infty$ and $E_n = E_\infty$. We first assume

$$\Delta \Omega_j = \Omega(E_{j+1}, \alpha_{j+1}) - \Omega(E_j, \alpha_j),$$

$$= O((\Delta \alpha)^2)$$

for large $n$. We then obtain

$$\Omega(E_0, \alpha_0) - \Omega(E_\infty, \alpha_\infty) = \lim_{n \to \infty} \sum_{j=1}^{n-1} O((\Delta \alpha)^2) ,$$

$$= \lim_{n \to \infty} O\left(\frac{1}{n}\right),$$

$$= 0.$$  

This shows the adiabatic theorem.

We next prove Eq. (3-16). Without loss of generality, we can assume that the value of $\alpha$ is monotonically changed from $\alpha_j$ to $\alpha_j + \Delta \alpha$. Defining the protocol of the parameter change $\alpha_t()$ as

$$\alpha_t(t) = \alpha_j + (\Delta \alpha)\frac{t}{\tau},$$

we calculate $\Delta \Omega_j$ from Eq. (3-10) in the following way:

$$\Delta \Omega_j = \lim_{\tau \to \infty} \int_0^\tau dt |\Sigma(t)| \delta A(t) \frac{d\alpha_t}{dt} ,$$

$$= \lim_{\tau \to \infty} \frac{(\Delta \alpha)}{\tau} \int_0^\tau dt |\Sigma(t)| \delta A(t).$$

When $\Delta \alpha$ is sufficiently small, $\Delta \Omega_j$ is evaluated as

$$\Delta \Omega_j = |\Sigma(0)| \lim_{\tau \to \infty} \frac{(\Delta \alpha)}{\tau} \int_0^\tau dt \delta A(t) + O((\Delta \alpha)^2) ,$$

$$= O((\Delta \alpha)^2),$$

where we have used

$$\lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau dt \delta A(t) = 0,$$

which is equivalent to

$$\lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau dt A(t) = \langle A \rangle_{\Sigma}.$$  

This equality holds for almost all initial conditions with respect to the Lebesgue measure on the energy surface because of the ergodicity with respect to the microcanonical measure.

(q.e.d)
3.2. Boltzmann entropy

We define the Boltzmann entropy $S_B$ as

$$S_B(\Sigma) = \log \Omega(\Sigma),$$  \hspace{1cm} (3.27)

where the Boltzmann constant is assumed to be the unity. For later convenience, we define the temperature $T(\Sigma)$ as

$$T(\Sigma) = \left( \frac{\partial S_B}{\partial E} \right)^{-1} = \frac{\Omega(\Sigma)}{|\Sigma|}.$$  \hspace{1cm} (3.28)

Although Eq. (3.27) is the formula which makes us possible to calculate the thermodynamic entropy for the equilibrium state $\Sigma$, we define the time evolution of $S_B$ as

$$S_B(t) = S_B(\Sigma(t)).$$  \hspace{1cm} (3.29)

Then, from Eqs. (3.10), (3.27) and (3.28), we obtain

$$\frac{dS_B}{dt} = \frac{1}{T(\Sigma)} \frac{\delta A}{\delta t}. \hspace{1cm} (3.30)$$

The integration of this equation during the time interval $[0, \tau]$ leads to

$$\Delta S_B = \int_0^\tau \frac{dQ_{qs}}{T} dt,$$  \hspace{1cm} (3.31)

Here, we notice that $\delta A$ equals to the energy change $\Delta E$ during a time interval $[t, t + dt]$ and that $\langle A \rangle_\Sigma d\alpha$ may be interpreted as the quasi-static work, $W_{qs}$, calculated under the condition that the system stays virtually in the energy surface. $W_{qs}$ is identical to the work done in the actual process which can be realized when the system contacts a heat bath with slowly changing temperature. The quasi-static heat $Q_{qs}$ from the heat bath is then given by

$$Q_{qs} = \Delta E - W_{qs} = \delta A d\alpha.$$  \hspace{1cm} (3.32)

Using $Q_{qs}$, we rewrite Eq. (3.31) as

$$\Delta S_B = \int_0^\tau \frac{dQ_{qs}}{T} dt,$$  \hspace{1cm} (3.33)

$$= \int_0^\tau \frac{dQ_{qs}}{T}.$$  \hspace{1cm} (3.34)

This should be compared with the Clausius’s formula

$$\Delta S = \int \frac{dQ}{T},$$  \hspace{1cm} (3.35)

where $d'Q$ is an infinitely small quasi-static heat exported from a heat bath. In this way, the Boltzmann entropy turns out to be identified to the thermodynamic entropy.

3.3. Entropy change for step processes

We discuss the step process given by

$$\frac{d\alpha}{dt} = \delta(t) \Delta \alpha.$$  \hspace{1cm} (3.36)

\* See page 371 in the Boltzmann’s book \(\text{[25]}\) as an explicit presentation of the Boltzmann formula. However, the expression of Eq. (3.27) was first proposed by Gibbs as the correspondence of thermodynamic entropy. See page 128 in the Gibbs’s book \(\text{[28]}\). The monograph by P. and T. Ehrenfest is also useful to know contemporary ideas with them. \(\text{[25]}\)

\** Do not confuse it with the time evolution of the $H$-function in the $H$-theorem of Boltzmann. \(\text{[25]}\)
In the argument below, \( \Sigma_0 = (E_0, \alpha_0) \) and \( \Sigma_1 = (E_1, \alpha_1) \) denote the initial and final states, respectively. By substituting Eq. (3.36) into Eq. (3.31), we have

\[
\Delta S_B = \frac{1}{2} \left[ \frac{\delta A(0_+)}{T(\Sigma_1)} + \frac{\delta A(0_-)}{T(\Sigma_0)} \right] \Delta \alpha,
\]

(3.37)

where note that \( \delta A \) and \( T \) are discontinuous at \( t = 0 \). We consider the average over initial conditions sampled from the microcanonical ensemble on the energy surface \( \Sigma_0 \). This average is denoted by \( \langle \rangle \). We calculate \( \langle S_B \rangle_0 \) as

\[
\langle S_B \rangle_0 = \langle (\Delta S_B) \rangle_0 = (\Delta \alpha)^2 \left[ \frac{\partial \Sigma}{\partial E} \left( \langle \delta A \rangle_0 \right) + \partial \langle \delta A \rangle_0 \right] + o((\Delta \alpha)^2),
\]

(3.38)

where \( T_0 = T(\Sigma_0) \). (The proof will be given below.) Further, since the evaluation

\[
\frac{\partial}{\partial E} \left( \langle \delta A \rangle_0 \right) = o(N)
\]

is expected when \( N \to \infty \), we obtain

\[
\langle S_B \rangle_0 = \frac{(\Delta \alpha)^2}{2T_0} \left[ \langle (\delta A) \rangle_0 \right]^2 + o(N, (\Delta \alpha)^2) > 0,
\]

(3.40)

where we have used

\[
\frac{1}{\Sigma} \frac{\partial \Sigma}{\partial E} = \frac{1}{T} + O\left( \frac{1}{N} \right).
\]

(3.41)

In the thermodynamic limit, \( \langle S_B \rangle_0 \) is equal to the entropy difference \( S_B(\Sigma_1) - S_B(\Sigma_0) \) for the most probable process \( \Sigma_0 \to \Sigma_1 \). Thus, we conclude

\[
S_B(\Sigma_1) \geq S_B(\Sigma_0) + o(N, (\Delta \alpha)^2)
\]

(3.42)

for the most probable step process \( \Sigma_0 \to \Sigma_1 \).

Furthermore, from Eq. (3.37), the fluctuation \( \langle (\Delta S_B) \rangle \) is calculated as

\[
\langle (\Delta S_B)^2 \rangle_0 = \frac{(\Delta \alpha)^2}{T_0^2} \langle (\delta A) \rangle_0^2 + o((\Delta \alpha)^2).
\]

(3.43)

Combing this result with Eq. (3.41), we obtain the equality

\[
\langle \Delta S_B \rangle_0 = \frac{1}{2} \langle (\Delta S_B)^2 \rangle_0 + o((\Delta \alpha)^2, N).
\]

(3.44)

This is the fluctuation-response relation for the entropy change.

Now, we prove Eq. (3.38).

(proof)

We first find

\[
\langle \left[ \frac{\delta A(0_+)}{T(\Sigma_1)} + \frac{\delta A(0_-)}{T(\Sigma_0)} \right] \rangle_0 = \frac{\langle \delta A(0_+) \rangle_0}{T_0} + o((\Delta \alpha)^2).
\]

(3.45)

From Eq. (3.37), we have

\[
\langle \Delta S_B \rangle_0 = \frac{\langle \delta A(0_+) \rangle_0 (\Delta \alpha) + o((\Delta \alpha)^3)}{2T_0}.
\]

(3.46)

Let us evaluate \( \langle \delta A(0_+) \rangle_0 \) up to the order of \( \Delta \alpha \), where

\[
\langle \delta A(0_+) \rangle_0 = \left\langle \frac{\partial H}{\partial \alpha} (\Gamma(0_+), \alpha(0_+)) \right\rangle_0 - \left\langle \frac{\partial H}{\partial \alpha} \right\rangle_{\Sigma_1}.
\]

(3.47)
Since $\Gamma(0_+) = \Gamma(0_-)$, we expand the first term of the right-hand side in such a way that

$$\frac{\partial H}{\partial \alpha}(\Gamma(0_+), \alpha(0_+)) = \frac{\partial H}{\partial \alpha}(\Gamma(0_-), \alpha(0_-)) + \frac{\partial^2 H}{\partial \alpha^2}(\Gamma(0_-), \alpha(0_-)) \Delta \alpha + O((\Delta \alpha)^2). \quad (3.48)$$

Taking the average over the initial conditions, we obtain

$$\langle \frac{\partial H}{\partial \alpha}(\Gamma(0_+), \alpha(0_+)) \rangle_0 = \langle \frac{\partial H}{\partial \alpha} \rangle_0 + \langle \frac{\partial^2 H}{\partial \alpha^2} \rangle_0 \Delta \alpha + O((\Delta \alpha)^2). \quad (3.49)$$

We next evaluate the second term of right-hand side of Eq. (3.47).

$$\langle \langle \frac{\partial H}{\partial \alpha} \rangle_{\Sigma_1} \rangle_0 = \langle \frac{1}{|\Sigma_1|} \int d\Gamma \frac{\partial H}{\partial \alpha} \delta(H(\Gamma, \alpha_1) - E_1) \rangle_0. \quad (3.50)$$

We notice that there are four terms which include $\Delta \alpha$. (i) $\Delta \alpha$ appears in $1/|\Sigma_1|$, (ii) it appears in $\partial H/\partial \alpha$ in the integrand, (iii) it appears in $H(\Gamma, \alpha_1)$ in the Dirac’s delta function, and (iv) it appears in $E_1$ in the Dirac’s delta function. We extract the contribution proportional to $\Delta \alpha$ in each term.

(i) The first term: The contribution is

$$- \frac{1}{|\Sigma_1|^2} \frac{d|\Sigma_1|}{d\alpha} \int d\Gamma \frac{\partial H}{\partial \alpha} \delta(H(\Gamma, \alpha_0) - E_0), \quad (3.51)$$

where we have defined

$$\frac{d}{d\alpha} = \frac{\partial}{\partial \alpha} + A \frac{\partial}{\partial E}. \quad (3.52)$$

We here note that the equality

$$\frac{d\Omega}{d\alpha} = 0. \quad (3.53)$$

holds owing to the adiabatic theorem. This equality and the relation $\Omega = |\Sigma|T$ leads to

$$\frac{d|\Sigma|}{d\alpha} = - \left| \frac{\Sigma_0}{T_0} \right| \frac{dT}{d\alpha} \bigg|_0. \quad (3.54)$$

Thus, Eq. (3.51) becomes

$$\frac{1}{T_0} \frac{\partial T}{\partial \alpha} \bigg|_0 \langle A \rangle_0. \quad (3.55)$$

(2) The second term: Without any calculation, the contribution from the second term is

$$\langle \frac{\partial^2 H}{\partial \alpha^2} \rangle_0. \quad (3.56)$$

(3) The third and forth terms: In deriving the third and forth terms, we employ the following formula

$$\int d\Gamma \delta'(H - E)f(\Gamma) = \int dE' \int_{H=E'} \frac{d\sigma}{|\nabla H|} \delta'(E' - E)f(\Gamma), \quad (3.57)$$

$$= -\frac{\partial}{\partial E'} \left[ \int_{H=E'} \frac{d\sigma}{|\nabla H|} f(\Gamma) \right]_{E'=E}, \quad (3.58)$$

$$= -\frac{\partial}{\partial E'} \left[ \langle f \rangle_{(E', \alpha)} |\Sigma(E', \alpha)| \right]_{E'=E}. \quad (3.59)$$
Owing to this formula, we calculate the contribution from the third term

\[
\frac{1}{|\Sigma|_0} \int d\Gamma \left( \frac{\partial H}{\partial \alpha} \right)^2 \delta' (H(\Gamma, \alpha_0) - E_0) \\
= -\frac{1}{|\Sigma|_0} \frac{\partial}{\partial E} \left[ \left( \frac{\partial H}{\partial \alpha} \right)^2 |\Sigma| \right] \bigg|_0,
\]

\[
= -\frac{\partial}{\partial E} \left( \frac{\partial H}{\partial \alpha} \right)^2 \bigg|_0 - \frac{1}{|\Sigma|_0} \frac{\partial |\Sigma|}{\partial E} \left( \frac{\partial H}{\partial \alpha} \right)^2 \bigg|_0.
\]

Similarly, the contribution from the forth term is obtained as

\[
-\frac{1}{|\Sigma|_0} \int d\Gamma \frac{\partial H}{\partial \alpha} \delta' (H(\Gamma, \alpha_0) - E_0) \left\langle \frac{\partial H}{\partial \alpha} \right\rangle_0 \\
= \frac{\partial}{\partial E} \left( \frac{\partial H}{\partial \alpha} \right)^2 \bigg|_0 + \frac{1}{|\Sigma|_0} \frac{\partial |\Sigma|}{\partial E} \left( \frac{\partial H}{\partial \alpha} \right)^2 \bigg|_0.
\]

The contributions from the third and forth terms are combined in the form

\[
-\frac{1}{|\Sigma|_0} \frac{\partial |\Sigma|}{\partial E} \bigg| \left( \delta A \right)^2 \bigg|_0 - \frac{\partial}{\partial E} \left( \delta A \right)^2 \bigg|_0 - \left\langle A \right\rangle_0 \frac{\partial \left\langle A \right\rangle_\Sigma}{\partial E} \bigg|_0.
\]

Then, all the contributions given by Eqs. (3.55), (3.56) and (3.66) are summarized as

\[
\left\langle \left( \frac{\partial H}{\partial \alpha} \right)^2 \right\rangle \Sigma_0 = \left\langle \frac{\partial H}{\partial \alpha} \right\rangle_0 + \left\langle \frac{\partial^2 H}{\partial \alpha^2} \right\rangle_0 - \frac{\partial}{\partial E} \left( \delta A \right)^2 \bigg|_0 \Delta \alpha - \frac{\partial}{\partial E} \left( \delta A \right)^2 \bigg|_0 \Delta \alpha,
\]

where we have used the equality

\[
\frac{1}{T} \frac{\partial T}{\partial \alpha} = \frac{\partial \left\langle A \right\rangle_\Sigma}{\partial E} = 0.
\]

(The proof of this equality will be given below.) The substitution of Eqs. (3.43) and (3.68) to Eq. (3.47) yields

\[
\left\langle \delta A(0_+) \right\rangle_0 = \frac{1}{\Sigma_0} \frac{\partial |\Sigma|}{\partial E} \left( \delta A \right)^2 \bigg|_0 \Delta \alpha + \frac{\partial}{\partial E} \left( \delta A \right)^2 \bigg|_0 \Delta \alpha + O((\Delta \alpha)^2).
\]

Recalling Eq. (3.46), we finally obtain Eq. (3.38). (q.e.d)

Here, the proof of Eq. (3.69) is shown. One may find that Eq. (3.69) is equivalent to a Maxwell’s relation.

(proof)

For simplicity, we use the abbreviation \( A \) for \( \left\langle A \right\rangle_\Sigma \). Then, \( A \) is a function of \((S_B, \alpha)\). Since we can write

\[
A = A(S_B, \alpha) = \left( \frac{\partial E}{\partial \alpha} \right)_{S_B},
\]

we calculate

\[
\left( \frac{\partial A}{\partial E} \right)_\alpha = \left( \frac{\partial A}{\partial S_B} \right)_\alpha \left( \frac{\partial S_B}{\partial E} \right)_\alpha,
\]

\[
= \frac{1}{T} \frac{\partial^2 E}{\partial S_B \partial \alpha},
\]

\[
= \frac{1}{T} \frac{\partial T}{\partial \alpha}.
\]
3.4. Remark

In this section, we have shown that $\Delta S_B$ is positive for most probable step processes. One may then ask whether or not $\Delta S_B$ is positive for arbitrary processes. As one example, one may evaluate $\Delta S_B$ near quasi-static processes based on several physical assumptions. However, if we consider this question from the definition of $\Delta S_B$, it seems hard to obtain any general results.

Nevertheless, since $S_B$ is equivalent to the thermodynamic entropy, we expect the inequality

$$\Delta S_B \geq o(N) \quad (3.75)$$

holds for most probable processes in general. We will discuss the validity of Eq. (3.75) in Section 6.2 based on Lyapunov analysis of chaotic systems. We now leave statistical mechanics and enter Lyapunov analysis.

§4. Lyapunov analysis

One of essential features of chaotic systems is the sensitivity of initial conditions. Consider a trajectory segment, $\{\Gamma(t), \ 0 \leq t \leq \infty\}$. Almost all trajectories starting from phase space points in a neighborhood at $\Gamma(0)$ separate exponentially in time from the trajectory $\Gamma()$. Such a behavior can be discussed quantitatively by measuring the expansion of vectors in the tangent spaces around the trajectory. More generally, we can discuss the time evolution of the $k$-dimensional volume element, which is given by the exterior product of $k$ independent vectors in the tangent space. (See Appendix for basic properties of the volume element and exterior product.) Such an argument includes the Liouville’s theorem as a special case ($k = 2N$), which states that the $2N$ dimensional volume element keeps its volume along the trajectory. From the observation for both the cases that $k = 1$ and $k = 2N$, we expect that the tangent space at each point is decomposed into subspaces associated with the expansion ratios.

Indeed, it has been known that the multiplicative ergodic theorem of Oseledets provides a mathematical description of the naive expectation. Nowadays, the analysis of tangent spaces, which is often referred to as Lyapunov analysis, becomes a standard technique to discuss chaos owing to the establishment of a numerical calculation method.

In this section, we pay attention to Hamiltonian systems without parameter change except for the final two subsections, and we review the Lyapunov analysis with emphasizing its computational aspects.

When the value of $\alpha$ is not changed in time, the evolution map from $t = t_0$ to $t = t_1$ takes a form $U_{t_1-t_0}$ and satisfies

$$\Gamma(t) = U_t(\Gamma(0)). \quad (4.1)$$

The change of the trajectory at time $t$, $\delta \Gamma(t)$, against infinitely small change of the initial condition, $\delta \Gamma(0)$, is written as

$$\delta \Gamma(t) = U_t(\Gamma(0) + \delta \Gamma(0)) - U_t(\Gamma(0)), \quad (4.2)$$

$$= T(t, \Gamma(0)) \delta \Gamma(0). \quad (4.3)$$

$T(t, \Gamma(0))$ is called the linearized evolution map and is calculated by numerical integration of the linearized evolution equation. Note that the matrix $T(t, \Gamma(0))$ is determined by the trajectory segment $\{\Gamma(t'), \ 0 \leq t' \leq t\}$. We analyze the matrix $T(t, \Gamma(0))$ below.

4.1. Gram-Schmidt decomposition

Let $\{e_i, \ 1 \leq i \leq 2N\}$ be a set of orthogonal unit vectors given randomly in the tangent space at $\Gamma(0)$. For a while, we will use the abbreviation $T$ for $T(t, \Gamma(0))$. Since almost all vectors expand toward the most unstable direction, the direction of the vector $Te_1$ may approach to the most unstable
direction when \( t \) is sufficiently large. We thus define a unit vector in the tangent space at \( \Gamma(t) \) as

\[
f_1 = \frac{\mathcal{T}e_1}{|\mathcal{T}e_1|}.
\] (4.4)

\( f_1 \) is expected to indicate the most unstable direction at \( \Gamma(t) \) when \( t \to \infty \). Similarly, we define the most unstable direction in the orthogonal co-space of \( f_1 \)

\[
f_2 = \frac{\mathcal{T}e_2 - (\mathcal{T}e_2, f_1) f_1}{|\mathcal{T}e_2 - (\mathcal{T}e_2, f_1)|}.
\] (4.5)

Repeating the similar consideration, we define the \( i \)-th unstable direction

\[
f_i = \frac{\mathcal{T}e_i - \sum_{j=1}^{i-1} (\mathcal{T}e_i, f_j) f_j}{|\mathcal{T}e_i - \sum_{j=1}^{i-1} (\mathcal{T}e_i, f_j) f_j|}.
\] (4.6)

Since \( \{f_i, 1 \leq i \leq 2N\} \) is a set of orthonormal unit vectors in the tangent space at \( \Gamma(t) \), we can find an orthogonal matrix \( \mathcal{F}(t, \Gamma(0)) \) given by

\[
f_i = \mathcal{F}(t, \Gamma(0)) e_i.
\] (4.7)

Further, from Eq. (4.6), \( \mathcal{T}e_i \) is written as

\[
\mathcal{T}(t, \Gamma(0))e_i = \sum_k L_{ik}(t, \Gamma(0)) \mathcal{F}(t, \Gamma(0)) e_k,
\] (4.8)

where \( L_{ij} \) is the \((i,j)\)-element of an lower triangle matrix \( \mathcal{L} \). Eq. (4.8) is the Gram-Schmidt decomposition of the matrix \( \mathcal{T} \). Since the diagonal element will be particularly important below, we write it explicitly as

\[
L_{ii} = |\mathcal{T}e_i - \sum_{j=1}^{i-1} (\mathcal{T}e_i, f_j) f_j|.
\] (4.9)

4.2. Convergence property

As mentioned above, \( f_i \) indicates the \( i \)-th unstable direction only when \( t \to \infty \). Let \( e_{i*}(\Gamma(t)) \) be the ‘true’ \( i \)-th unstable direction at \( \Gamma(t) \). In order to have \( e_{i*}(\Gamma(t)) \) within a certain accuracy, we need to confirm

\[
d(\mathcal{F}(t, \Gamma(0)) e_i, e_{i*}(\Gamma(t))) \leq \epsilon,
\] (4.10)

where \( \epsilon \) is a small number related to the accuracy we require, and \( d(e, e') \) is the absolute value of the sine of the angle between two unit vectors \( e \) and \( e' \).

\[
d(e, e') = \sqrt{1 - (e, e')^2}.
\] (4.11)

However, since we do not have \( e_{i*}(\Gamma(t)) \) yet, we cannot confirm whether or not Eq. (4.10) is satisfied. Then, instead of Eq. (4.10), we check the condition

\[
d(\mathcal{F}(t, \Gamma(0)) e_i, \mathcal{F}(t, \Gamma(0)) e_i') \leq \epsilon
\] (4.12)

for two sets of orthogonal unit vectors \( \{e_i, 1 \leq i \leq 2N\} \) and \( \{e_i', 1 \leq i \leq 2N\} \) which are made randomly. When Eq. (4.12) is satisfied, we assume that the true \( i \)-th unstable direction is determined by

\[
e_{i*}(\Gamma(t)) \simeq \mathcal{F}(t, \Gamma(0)) e_i
\] (4.13)

within an accuracy we require.

When we numerically obtain \( e_{i*}(\Gamma(0)) \) at an arbitrary point \( \Gamma(0) \), we consider a trajectory segment \( \{\Gamma(t), -t_b \leq t \leq 0\} \) and check the condition

\[
d(\mathcal{F}(t_b, \Gamma(-t_b)) e_i, \mathcal{F}(t_b, \Gamma(-t_b)) e_i') \leq \epsilon,
\] (4.14)
for sufficiently large \( t_b \). When Eq. (1.14) is satisfied, we assume
\[
e_{si}(\Gamma(0)) \simeq \mathcal{F}(t_b, \Gamma(-t_b)) e_i
\] (4.15)
within an accuracy we require.

We do not know a mathematical condition under which Eq. (4.12) is satisfied. In the argument below, we assume that Eq. (4.12) is satisfied and that a set of vectors \( \{e_{si}(\Gamma(t))\} \) is determined for an arbitrary point \( \Gamma \). Once \( e_{si}(\Gamma(0)) \) is determined, \( e_{si}(\Gamma(t)) \) is calculated by
\[
e_{si}(\Gamma(t)) = \mathcal{F}(t, \Gamma(0)) e_{si}(\Gamma(0)).
\] (4.16)

4.3. Lyapunov vectors

So far, we have stated that \( e_{si}(\Gamma(t)) \) indicates the \( i \)-th unstable direction at \( \Gamma(t) \). More precisely, \( e_{si}(\Gamma(t)) \) indicates the most unstable direction in the orthogonal co-space of the subspace spanned by \( \{e_{sj}(\Gamma(t))\}, 1 \leq j \leq i - 1 \} \) in the tangent space at \( \Gamma(t) \). The term orthogonal co-space in this statement leads to a non-favorable property of \( e_{si}(\Gamma(t)) \): \( e_{si}(\Gamma(t)) \) does not satisfy
\[
\mathcal{T}(t, \Gamma(0)) e_{si}(\Gamma(0)) \propto e_{si}(\Gamma(t))
\] (4.17)
except for the case \( i = 1 \). This seems a little bit strange, because the unstable nature should be defined as something consistent along the trajectory. Then, we define a set of vectors \( \{\xi_i(\Gamma(t)), 1 \leq i \leq 2N\} \) which satisfies the two conditions. The first condition is the transitivity
\[
\mathcal{T}(t, \Gamma(0)) \xi_i(\Gamma(0)) \propto \xi_i(\Gamma(t)),
\] (4.18)
and the second condition is that the vector space generated by \( \{e_{sj}, 1 \leq j \leq i\} \) is spanned by \( \{\xi_j, 1 \leq j \leq i\} \). The second condition is expressed by
\[
\sum_j A_{ij} \xi_j(\Gamma(t)) = e_{si}(\Gamma(t)),
\] (4.19)
where \( A_{ij} = 0 \) for \( i < j \), and \( A_{ij} \) is regarded as the \((ij)\)-element of a lower triangle matrix \( A \).

Now, we define the \( i \)-th expansion factor \( A_i(t, \Gamma(0)) \) in the \( i \)-th unstable direction
\[
\mathcal{T}(t, \Gamma(0)) \xi_i(\Gamma(0)) = A_i(t, \Gamma(0)) \xi_i(\Gamma(t)).
\] (4.20)
We call \( \xi_i \) the \( i \)-th Lyapunov vector. In order to determine uniquely the value of \( A_i \), we assume the normalization condition that the volume of the parallelepiped made by \( \{\xi_j, 1 \leq j \leq i\} \) is the unity. This condition is expressed by
\[
| \wedge_{j=1}^i \xi_j | = 1
\] (4.21)
for \( 1 \leq i \leq 2N \). (See Appendix.) We also assume that \( A_{ii} \) is positive. Under these conditions, we can prove that the \( i \)-th expansion factor \( A_i(t, \Gamma(0)) \) is calculated by the Gram-Schmidt decomposition Eq. (1.8) with \( e_{si}(\Gamma(0)) \).

(proof)
From Eq. (1.8), we have
\[
\mathcal{T}(t, \Gamma(0)) e_{si}(\Gamma(0)) = \sum_k L_{ik}(t, \Gamma(0)) \mathcal{F}(t, \Gamma(0)) e_{sk}(\Gamma(0)).
\] (4.22)
Using Eqs. (4.19) and (4.20), we rewrite the left-hand side of Eq. (4.22) as
\[
\sum_j A_{ij}(\Gamma(0)) \mathcal{T}(t, \Gamma(0)) \xi_j(\Gamma(0))
\] (4.23)
\[
= \sum_j A_{ij}(\Gamma(0)) A_j(t, \Gamma(0)) \xi_j(\Gamma(t))
\] (4.24)
\[
= \sum_{jk} A_{ij}(\Gamma(0)) A_j(t, \Gamma(0))(A(\Gamma(t))^{-1})_{jk} e_{sk}(\Gamma(t))
\] (4.25)
\[
= \sum_{jk} A_{ij}(\Gamma(0)) A_j(t, \Gamma(0))(A(\Gamma(t))^{-1})_{jk} \mathcal{F}(t, \Gamma(0)) e_{sk}(\Gamma(0)).
\] (4.26)
Comparing the right-hand side of Eq. (4.22) and Eq. (4.26), we find

\[ L_{ik}(t, \Gamma(0)) = \sum_j A_{ij}(\Gamma(0))A_j(t, \Gamma(0))(\Lambda(\Gamma(t))^{-1})_{jk}. \]  

(4.27)

Further, from Eqs. (4.19) and (4.21), we can easily see

\[ |A_{ii}| = 1 \]  

(4.28)

for \( 1 \leq i \leq 2N \). (See Appendix.) Since \( A_{ii} \) is assumed to be positive, \( A_{ii} = 1 \). Then, Eq. (4.27) yields

\[ \Lambda_i(t, \Gamma(0)) = L_{ii}(t, \Gamma(0)). \]  

(4.29)

In this way, the \( i \)-th expansion factor can be calculated numerically.

4.4. Lyapunov exponent

The \( i \)-th expansion ratio \( \lambda_i(\Gamma(t)) \) at \( \Gamma(t) \) is defined as

\[ \frac{d\Lambda_i(t, \Gamma(0))}{dt} = \lambda_i(\Gamma(t))A_i(t, \Gamma(0)). \]  

(4.30)

The long time average of the \( i \)-th expansion ratio \( \lambda_i(\Gamma(t)) \) is called the \( i \)-th Lyapunov exponent, which is given by

\[ \bar{\lambda}_i = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau dt \lambda_i(\Gamma(t)), \]  

(4.31)

\[ = \lim_{\tau \to \infty} \frac{1}{\tau} \log \Lambda_i(\tau, \Gamma(0)). \]  

(4.32)

\( \bar{\lambda}_i \) is sometimes called the 'local' Lyapunov exponent because \( \bar{\lambda}_i \) depends on \( \Gamma(0) \). However, from the ergodic theorem, \( \lambda_i \) has a same value for almost all \( \Gamma(0) \) with respect to the microcanonical measure. Since we assume the ergodicity of the microcanonical measure, we do not take care of the local nature of the Lyapunov exponent.

As clearly seen from the method of construction of Lyapunov vectors, we find

\[ \bar{\lambda}_1 \geq \bar{\lambda}_2 \cdots \geq \bar{\lambda}_{2N}. \]  

(4.33)

In Hamiltonian systems, there are at least two zero Lyapunov exponents whose Lyapunov vectors indicate the normal direction of the energy surface and the tangential direction of the trajectory. In the argument below, we assume that there are \( N_p \) positive Lyapunov exponents. Unless the system has a further conservation law such as momentum conservation, \( N_p \) equals to \( N - 1 \).

The information loss rate at \( \Gamma(t) \), \( h(\Gamma(t)) \), is defined as the sum of the expansion ratios with the positive Lyapunov exponents.

\[ h(\Gamma(t)) = \sum_{\lambda_i > 0}^{\lambda_i > 0} \lambda_i(\Gamma(t)), \]  

(4.34)

\[ = \sum_{i=1}^{N_p} \lambda_i(\Gamma(t)). \]  

(4.35)

Notice that \( h(\Gamma(t)) \) represents the volume expansion ratio of the \( N_p \)-dimensional unstable space. That is, \( h(\Gamma(t)) \) is rewritten as

\[ h(\Gamma(t)) = \frac{d}{dt} \log \left| \bigwedge_{i=1}^{N-1} T(t, \Gamma(0)) \xi_i(\Gamma(0)) \right|. \]  

(4.36)

The long time average of the information loss rate, \( \bar{h} \), has the same value for almost all initial conditions with respect to the microcanonical measure. It has been known that \( \bar{h} \) is identical to the Kolmogorov-Sinai entropy when the system is hyperbolic. [31]
4.5. Contraction ratio

Let us recall that the expansion factor $\Lambda_i$ is calculated by the Gram-Schmidt decomposition under the normalization condition Eq. (4.21). However, this normalization lacks the balance between the unstable and stable directions. Since Hamiltonian systems possess a time reverse symmetry, such unbalance will cause theoretical complicatedness. In order to recover the symmetry, we introduce a new set of vectors $\{\xi_i^{(s)}, 1 \leq i \leq 2N\}$ given by

$$\xi_i^{(s)} = c_i \xi_{2N-i+1},$$  \hfill (4.37)

where $c_i$ is a positive number determined so as to satisfy

$$| \langle \xi_j^{(s)} \rangle_i | = 1$$ \hfill (4.38)

for $1 \leq i \leq 2N$. The set of vectors $\{\xi_i^{(s)}, 1 \leq i \leq 2N\}$ is made to respect stable directions from the most stable one.

We now define the contraction factor $\Lambda_i^{(s)}$ and contraction ratio $\lambda_i^{(s)}$ as

$$T(t, \Gamma(0)) \xi_i^{(s)}(\Gamma(0)) = \frac{1}{\Lambda_i^{(s)}(t, \Gamma(0))} \xi_i^{(s)}(\Gamma(t)), \quad \lambda_i^{(s)}(\Gamma(t)) = \frac{d}{dt} \log \Lambda_i^{(s)}(t, \Gamma(0)).$$  \hfill (4.39)

As will be seen in the next section, the contraction ratio is related to the expansion ratio of the time-reversed trajectory and this relation plays a role in simplifying arguments. In particular, the following estimation will be utilized.

$$\sum_{i=1}^{N_p} \lambda_{2N+1-i}(t) = -\sum_{i=1}^{N_p} \lambda_i^{(s)}(\Gamma(0)) + \frac{d}{dt} \sigma(N).$$  \hfill (4.40)

Here, the last term represents the time derivative of a function whose value is much smaller than $N$ when $N \to \infty$. Note that the left-hand side and the first term of the right-hand side are the order of $N$.

(proof)

Substituting Eq. (4.37) into Eq. (4.39), we have

$$c_i(\Gamma(0)) A_{2N+1-i}(t, \Gamma(0)) = \frac{1}{\Lambda_i^{(s)}(t, \Gamma(0))} c_i(\Gamma(t)).$$  \hfill (4.41)

The time derivative of the logarithm of the both-hand sides yields

$$\lambda_{2N+1-i}(\Gamma(t)) = -\lambda_i^{(s)}(\Gamma(t)) + \frac{d}{dt} \log \left( \frac{c_i(\Gamma(t))}{c_i(\Gamma(0))} \right).$$  \hfill (4.42)

We thus obtain

$$\sum_{i=1}^{N_p} \lambda_{2N+1-i}(\Gamma(t)) = -\sum_{i=1}^{N_p} \lambda_i^{(s)}(\Gamma(t)) + \frac{d}{dt} \sum_{i=1}^{N_p} \log \left( \frac{c_i(\Gamma(t))}{c_i(\Gamma(0))} \right).$$  \hfill (4.43)

Let us evaluate the second term of the right-hand side of Eq. (4.44). We first define an 'angle' $\phi_i$ as

$$| \langle \xi_j^{2N} \rangle_i | = | \langle \xi_j^{2N-i} \rangle_i | \langle \xi_j^{2N} \rangle_{2N+1-i} | \sin \phi_i,$$  \hfill (4.45)

where $0 \leq \phi_i \leq \pi/2$. (See Appendix.) By using the normalization condition of $\{\xi_i\}$, we rewrite Eq. (4.45) as

$$| \langle \xi_j^{2N} \rangle_{2N+1-i} \sin \phi_i = 1.$$  \hfill (4.46)
Using Eqs. (4.37) and (4.38), we obtain

$$c_1 \cdots c_t = \sin \phi_i.$$  \hspace{1cm} (4.47)

This leads to

$$\sum_{i=1}^{N_p} \log \left( \frac{c_i(\Gamma(t))}{c_i(\Gamma(0))} \right) = \log \left( \frac{\sin \phi_{N_p}(\Gamma(t))}{\sin \phi_{N_p}(\Gamma(0))} \right) = o(N),$$  \hspace{1cm} (4.48)

where we have assumed

$$\sin(\phi_{N_p}(\Gamma)) \gg O(\exp(-N)),$$  \hspace{1cm} (4.49)

which may be ensured by the condition that the unstable and stable manifolds intersect transversally.

**4.6. Weight on trajectory segments**

We consider a weight on the trajectory segment \(\{\Gamma(t), 0 \leq t \leq \tau\}\). The weight, \(W(\{\Gamma(t), 0 \leq t \leq \tau\})\), is a conditional probability finding trajectory segments remaining in a small tube around \(\{\Gamma(t), 0 \leq t \leq \tau\}\) when the initial condition is chosen in a small region around \(\Gamma(0)\). More explicitly, the weight \(W\) is defined in the following way.

Substitute that the phase space is decomposed into small cells \(\{\Delta_j\}\) with a sufficiently small size \(\epsilon\) and that \(\Gamma(0)\) is included in the \(i\)-th cell \(\Delta_i\). Then, the number of cells which intersect with \(U_\tau(\Delta_i)\), \(N(\tau, \epsilon)\), can be counted. We can choose the value of \(\epsilon\) so that the region \(U_\tau(\Delta_i)\) remains in a linear regime around \(U_\tau(\Gamma(0))\). This condition may be given by

$$\epsilon \ll \epsilon_c(\tau),$$  \hspace{1cm} (4.50)

where the value of \(\epsilon_c(\tau)\) is determined by nonlinear properties of dynamical systems. Under this condition, \(N(\tau, \epsilon)\) measures the number of distinguishable trajectory segments starting from the neighborhood of \(\Gamma(0)\). Therefore, we define the weight as

$$W(\{\Gamma(t), 0 \leq t \leq \tau\}) = \frac{1}{N(\tau, \epsilon)}.$$  \hspace{1cm} (4.51)

Then, we can show

$$W(\{\Gamma(t), 0 \leq t \leq \tau\}) = | \bigwedge_{i=1}^{N_p} T(-\tau, \Gamma(\tau)) \xi_i(\Gamma(\tau)) |$$  \hspace{1cm} (4.52)

in an appropriate limit of large \(\tau\) and small \(\epsilon\). (Since \(\epsilon_c(\tau) \to 0\) for the limit \(\tau \to \infty\), we need to take care of a delicate problem of double limits. Nevertheless, we assume simply that we can choose an appropriate asymptotic limit.)

(proof)

Consider the time evolution of a small region \(\Delta_i\). The region expands and contracts in the unstable and stable directions, respectively. After a sufficiently long time, the region almost collapses into the \(N_p\)-dimensional unstable manifold, and intersects with cells in the unstable directions. Since the \(N_p\)-dimensional volume element in the unstable manifold at \(\Gamma(\tau)\) is written as \(\bigwedge_{i=1}^{N_p} \xi_i(\Gamma(\tau))\), we expect

$$N(\tau, \epsilon) = \frac{| \bigwedge_{i=1}^{N_p} \xi_i(\Gamma(\tau)) |}{| \bigwedge_{i=1}^{N_p} T(-\tau, \Gamma(\tau)) \xi_i(\Gamma(\tau)) |} = | \bigwedge_{i=1}^{N_p} T(-\tau, \Gamma(\tau)) \xi_i(\Gamma(\tau)) |^{-1}$$  \hspace{1cm} (4.53)

in an appropriate limit of large \(\tau\) and small \(\epsilon\). Substituting this into Eq. (4.51) leads to Eq. (4.52).

(q.e.d)

Further, by the relation Eqs. (4.30), Eq. (4.52) becomes a simpler form

$$W(\{\Gamma(t), 0 \leq t \leq \tau\}) = \exp(- \int_0^\tau d\theta(\Gamma(t))).$$  \hspace{1cm} (4.55)
4.7. Time dependent case

To this point in this section, we have assumed that the value of $\alpha$ is not changed in time. In this subsection, we briefly discuss Lyapunov analysis for systems with a time dependent parameter. When the value of $\alpha$ depends on $t$, the evolution map from $t = t_0$ to $t = t_1$ depends on the absolute time $t_0$ and $t_1$. Therefore, it takes the form $U_{t_1,t_0}$, and the linearized evolution map is written as $\mathcal{T}(t_1,t_0;\Gamma(t_0))$.

The Lyapunov analysis in such a case may be reconsidered carefully. However, we do not need general arguments. In the systems in question, the value of $\alpha$ is changed during a finite time interval $[\tau_i, \tau_f]$, where $0 \ll \tau_i \leq \tau_f \ll \tau$. Therefore, for example, the $i$-th Lyapunov vectors at $\Gamma(0)$ and $\Gamma(\tau)$ can be defined as $\xi_i(\Gamma(0))$ and $\xi_i(\Gamma(\tau))$, respectively.

Although the expansion factors, Lyapunov exponents and information loss rate do not make a sense in general, the argument on the weight $W$ is still valid. We can write

$$W(\{\Gamma(t), 0 \leq t \leq \tau\}) = | \wedge_{i=1}^{N_p} \mathcal{T}(0, \tau; \Gamma(\tau))\xi_i(\Gamma(\tau))|.$$  \hfill (4.56)

for sufficiently large $\tau$ and small $\epsilon$. We also define the actual information loss rate as the generalization of Eq. (4.36)

$$h_a(t,\Gamma(0)) = \frac{d}{dt} \log | \wedge_{i=1}^{N-1} \mathcal{T}(t, 0; \Gamma(0))\xi_i(\Gamma(0))|. \hfill (4.57)$$

4.8. Liouville’s theorem

In this subsection, we review a proof of the Liouville’s theorem which states that the $2N$-dimensional volume element keeps its volume along the trajectory. It is important to understand that the Liouville’s theorem holds even when the value of $\alpha$ is changed in time.

(proof)

We have the Hamiltonian equation

$$\frac{d\Gamma(t)}{dt} = -\mathcal{J} \left. \frac{\partial H(\Gamma, \alpha(t))}{\partial \Gamma} \right|_{\Gamma = \Gamma(t)}.$$  \hfill (4.58)

(See Eq. (2.8) in Section 2.) Since the linearized evolution equation is written as

$$\frac{d\delta\Gamma(t)}{dt} = -\mathcal{J} \left. \frac{\partial^2 H(\Gamma, \alpha(t))}{\partial \Gamma \partial \Gamma} \right|_{\Gamma = \Gamma(t)} \delta\Gamma(t), \hfill (4.59)$$

the linearized evolution map $\mathcal{T}(t, 0; \Gamma(0))$ satisfies the equation

$$\frac{d\mathcal{T}}{dt} = -\mathcal{J} \mathcal{B} \mathcal{T}, \hfill (4.60)$$

where $\mathcal{B}$ is a symmetric matrix. We then obtain

$$\frac{d(\mathcal{J}^\dagger \mathcal{J})}{dt} = \frac{d\mathcal{T}}{dt} \mathcal{J}^\dagger + \mathcal{J}^\dagger \frac{d\mathcal{T}}{dt} = -(\mathcal{J}^\dagger \mathcal{B} \mathcal{J}^\dagger \mathcal{J} \mathcal{J}^\dagger \mathcal{B} \mathcal{T}) \hfill (4.61)$$

$$= 0,$$ \hfill (4.62)

where we have used the equality

$$\mathcal{J}^\dagger \mathcal{J} = -\mathcal{J} \mathcal{J} = 1.$$ \hfill (4.64)

Since $\mathcal{T}(0, 0; \Gamma(0)) = 1$, Eq. (4.63) leads to

$$\mathcal{T}^\dagger \mathcal{J} \mathcal{J} = \mathcal{J}.$$ \hfill (4.65)

The determinant of the both-hand sides gives

$$\det[\mathcal{T}^\dagger \mathcal{T}] = 1.$$ \hfill (4.66)
Let \( \{e_i, 1 \leq i \leq 2N\} \) be an orthogonal set of unit vectors defined in the tangent space at \( \Gamma(0) \). The time evolution of the \( 2N \)-dimensional volume element \( \wedge_{i=1}^{2N} T e_i \) is given by \( \wedge_{i=1}^{2N} T e_i \), and its volume is calculated as

\[
| \wedge_{i=1}^{2N} T e_i | = \sqrt{\det TT^\dagger}
\]

(4.67)

(4.68)

(See Appendix.) Therefore, the \( 2N \)-dimensional volume element keeps its volume along the trajectory. (q.e.d.)

Further, using the Liouville’s theorem, we can prove that the equality

\[
\sum_{i=1}^{2N} \lambda_i(\Gamma(t)) = 0
\]

holds when the value of \( \alpha \) is not changed in time.

(proof)

Since the the value of \( \alpha \) is not changed in time, we obtain

\[
\sum_{i=1}^{2N} \lambda_i(\Gamma(t)) = \frac{d}{dt} \log \sum_{i=1}^{2N} \Lambda_i(t, \Gamma(0))
\]

(4.70)

\[
= \frac{d}{dt} \log | \wedge_{i=1}^{2N} T(t, \Gamma(0)) \xi_i(\Gamma(0)) |
\]

(4.71)

\[
= 0
\]

(4.72)

where the Liouville’s theorem is used to obtain the last line. (q.e.d)

§5. Reversibility

5.1. Reversibility in time evolution

We define a matrix \( R \) as

\[
(R \Gamma)_i = q_i,
\]

(5.1)

\[
(R \Gamma)_{i+N} = -p_i,
\]

(5.2)

where \( 1 \leq i \leq N \). The matrix \( R \) corresponds to the time reverse operator acting on the phase space point. We assume that the Hamiltonian under consideration possesses the time reverse symmetry

\[
H(R \Gamma, \alpha) = H(\Gamma, \alpha).
\]

(5.3)

Let \( U_{t,0} \) and \( \tilde{U}_{t,0} \) be the evolution maps for Hamiltonian equations with \( \alpha() \) and \( \tilde{\alpha}() \), respectively, where we have defined the time-reversed protocol of the parameter change \( \tilde{\alpha}() \) as

\[
\tilde{\alpha}(t) = \alpha(-t).
\]

(5.4)

Then, owing to the symmetry property Eq. (5.3), the identity

\[
U_{t,0} = R \tilde{U}_{-t,0} R.
\]

(5.5)

holds.

(proof)

Let \( \{\Gamma(t)\} \) and \( \{\tilde{\Gamma}(t)\} \) be trajectories given by

\[
\Gamma(t) = U_{t,0}(\Gamma(0)),
\]

(5.6)

\[
\tilde{\Gamma}(t) = \tilde{U}_{t,0}(\tilde{\Gamma}(0)),
\]

(5.7)
where \( \Gamma(0) \) and \( \tilde{\Gamma}(0) \) are the initial conditions which satisfy the relation
\[
\tilde{\Gamma}(0) = \mathcal{R}\Gamma(0). \tag{5.8}
\]

From Eq. (5.7), we obtain
\[
-\frac{d\tilde{\Gamma}(-t)}{dt} = -\mathcal{J} \frac{\partial H(\Gamma, \tilde{\alpha}(-t))}{\partial \Gamma} \bigg|_{\Gamma=\tilde{\Gamma}(-t)}, \tag{5.9}
\]
\[
= -\mathcal{J} \frac{\partial H(\Gamma, \alpha(t))}{\partial \Gamma} \bigg|_{\Gamma=\tilde{\Gamma}(-t)}, \tag{5.10}
\]
where we have used the equation of motion in the form Eq. (2.8) with the matrix \( \mathcal{J} \) satisfying Eq. (2.9). On the other hand, Eq. (5.6) leads to
\[
\mathcal{R} \frac{d\Gamma(t)}{dt} = -\mathcal{J} \frac{\partial H(\Gamma, \alpha(t))}{\partial \Gamma} \bigg|_{\Gamma=\Gamma(t)}, \tag{5.11}
\]
\[
= \mathcal{J} \frac{\partial H(\Gamma, \alpha(t))}{\partial (\mathcal{R}\Gamma)} \bigg|_{\Gamma=\Gamma(t)}, \tag{5.12}
\]
\[
= \mathcal{J} \frac{\partial H(\mathcal{R}\Gamma, \alpha(t))}{\partial (\mathcal{R}\Gamma)} \bigg|_{\Gamma=\Gamma(t)}, \tag{5.13}
\]
\[
= \mathcal{J} \frac{\partial H(\mathcal{R}\Gamma, \alpha(t))}{\partial \Gamma} \bigg|_{\Gamma=\mathcal{R}\Gamma(t)}, \tag{5.14}
\]
\[
= \mathcal{J} \frac{\partial H(\Gamma, \alpha(t))}{\partial \Gamma} \bigg|_{\Gamma=\mathcal{R}\Gamma(t)}. \tag{5.15}
\]

Here, the second line is obtained by the relation
\[
\mathcal{R}\mathcal{J} + \mathcal{J}\mathcal{R} = 0, \tag{5.16}
\]
the third line is derived from the relation \( \mathcal{R}\mathcal{R} = 1 \), and the equality of the forth line comes from the symmetry property Eq. (5.3).

Comparing Eqs. (5.10) and (5.15), we find that \( \tilde{\Gamma}(-t) \) and \( \mathcal{R}\Gamma(t) \) obey the same evolution equation. Recalling the relation for the initial condition in Eq. (5.8), we conclude
\[
\tilde{\Gamma}(0) = \mathcal{R}\Gamma(0) \tag{5.17}
\]
By using Eqs. (5.6) and (5.7), Eq. (5.17) is rewritten as
\[
\tilde{U}_{-t,0}(\mathcal{R}\Gamma(0)) = \mathcal{R}U_{t,0}(\Gamma(0)). \tag{5.18}
\]
Since \( \Gamma(0) \) is arbitrary, Eq. (5.15) holds.

In the argument below, \( \tilde{\Gamma}(t) \) will be assumed to be given by Eq. (5.17).

5.2. Reversibility in Lyapunov analysis

First, from Eq. (5.5), we have
\[
\mathcal{T}(t, 0; \Gamma(0)) = \mathcal{R}\tilde{T}(-t, 0; \tilde{\Gamma}(0))\mathcal{R}, \tag{5.19}
\]
where \( \mathcal{T}(t, 0; \Gamma(0)) \) and \( \tilde{T}(t, 0; \tilde{\Gamma}(0)) \) are the linearized evolution maps around the trajectories \( \Gamma() \) and \( \tilde{\Gamma}() \). In particular, when the value of \( \alpha \) is not changed, the equality \( \tilde{T} = \mathcal{T} \) holds. We then prove the identities
\[
\xi_i(\Gamma) = \mathcal{R}\xi^{(s)}_i(\mathcal{R}\Gamma), \tag{5.20}
\]
\[
\lambda_i(\Gamma) = \lambda^{(s)}_i(\mathcal{R}\Gamma), \tag{5.21}
\]
\[
h(\Gamma(t)) - h(\tilde{\Gamma}(-t)) = \frac{d}{dt}o(N). \tag{5.22}
\]
(proof)
Using the matrices defined as
\[ X_{ij}(\Gamma) = (\xi_j(\Gamma))_i, \]  
\[ X_{ij}^{(s)}(\Gamma) = (\xi_j^{(s)}(\Gamma))_i, \]  
we can write \( T(t, \Gamma(0)) \) in the two forms
\[ T(t, \Gamma(0)) = X(\Gamma(t))M(t, \Gamma(0))X(\Gamma(0))^{-1}, \]  
\[ T(t, \Gamma(0)) = X^{(s)}(\Gamma(t))M^{(s)}(t, \Gamma(0))X^{(s)}(\Gamma(0))^{-1}, \]  
where \( M(t, \Gamma(0)) \) and \( M^{(s)}(t, \Gamma(0)) \) are diagonal matrices whose \((i,i)\)-elements are given by \( \Lambda_i(t, \Gamma(0)) \) and \( \Lambda_i^{(s)}(t, \Gamma(0))^{-1} \), respectively. Using Eq. (5.26), we rewrite the right-hand side of Eq. (5.19) as
\[ RX_{ij}^{(s)}(\tilde{\Gamma}(-t))M_{ij}^{(s)}(-t, \tilde{\Gamma}(0))X_{ij}^{(s)}(\tilde{\Gamma}(0))^{-1}R, \]  
\[ = RX_{ij}^{(s)}(\tilde{\Gamma}(t))M_{ij}^{(s)}(-t, \tilde{\Gamma}(0))X_{ij}^{(s)}(\tilde{\Gamma}(0))^{-1}R, \]  
where we have used \( \tilde{\Gamma} = T \). Comparing Eq. (5.28) with the right-hand side of Eq. (5.25), we obtain
\[ X(\Gamma) = RX^{(s)}(\tilde{\Gamma}), \]  
\[ M(t, \Gamma(0)) = M^{(s)}(-t, \tilde{\Gamma}(0)), \]  
where notice the normalization conditions of \( \xi_i \) and \( \xi_i^{(s)} \) given by Eqs. (4.21) and (4.38).

Equation (5.29) is equivalent to Eq. (5.20), and Eq. (5.30) leads to Eq. (5.21), because of the equality
\[ \frac{d}{dt} \log \Lambda_i^{(s)}(-t, \tilde{\Gamma}(0))^{-1} = \lambda_i^{(s)}(\tilde{\Gamma}(-t)), \]  
\[ = \lambda_i^{(s)}(\tilde{\Gamma}(t)). \]  
Furthermore, \( h(\Gamma(t)) \) is expressed in terms of \( \{\lambda_i^{(s)}\} \) in the following way.
\[ h(\Gamma(t)) = \sum_{i=1}^{N_p} \lambda_i(\Gamma(t)), \]  
\[ = - \sum_{i=1}^{N_p} \lambda_{2N+i-1}(\Gamma(t)), \]  
\[ = \sum_{i=1}^{N_p} \lambda_i^{(s)}(\Gamma(t)) + \frac{d}{dt} \alpha(N), \]  
where the second and third lines come from Eqs. (4.69) and Eq. (4.41), respectively. On the other hand, from the symmetry property Eq. (5.21), \( h(\tilde{\Gamma}(-t)) \) is written as
\[ h(\tilde{\Gamma}(-t)) = \sum_{i=1}^{N_p} \lambda_i(\tilde{\Gamma}(-t)), \]  
\[ = \sum_{i=1}^{N_p} \lambda_i(\tilde{\Gamma}(t)), \]  
\[ = \sum_{i=1}^{N_p} \lambda_i^{(s)}(\Gamma(t)). \]
Comparing Eqs. (5.35) and (5.38), we obtain Eq.(5.22).

Using these identities, we can express the weight on the trajectory segment by the actual information loss of the time reversed trajectory

\[ W(\{\Gamma(t), \ 0 \leq t \leq \tau\}) = \int_0^\tau dt \tilde{h}_a(-t, \tilde{\Gamma}(-\tau)) \exp(o(N)), \quad (5.39) \]

where the actual information loss rate along the time-reversed trajectory \( \tilde{h}_a \) is defined as

\[ \tilde{h}_a(t, \tilde{\Gamma}(-\tau)) = \frac{d}{dt} \log | \wedge_{i=1}^{N_p} \mathcal{T}(t, -\tau; \Gamma(-\tau)) \xi_i(\tilde{\Gamma}(-\tau)) |. \quad (5.40) \]

(prove)

Let us recall the expression of the weight Eq. (5.54).

\[ W(\{\Gamma(t), \ 0 \leq t \leq \tau\}) = | \wedge_{i=1}^{N_p} \mathcal{T}(0, \tau; \Gamma(\tau)) \xi_i(\Gamma(\tau)) |. \quad (5.41) \]

The right-hand side is rewritten in the following way

\[ | \wedge_{i=1}^{N_p} \mathcal{R} \mathcal{T}(0, -\tau; \tilde{\Gamma}(-\tau)) \mathcal{R} \xi_i^{(s)}(\mathcal{R} \Gamma(\tau)) | = | \wedge_{i=1}^{N_p} \mathcal{T}(0, -\tau; \tilde{\Gamma}(-\tau)) \xi_i^{(s)}(\tilde{\Gamma}(-\tau)) | = | \wedge_{i=1}^{N_p} \mathcal{T}(0, -\tau; \tilde{\Gamma}(-\tau)) \xi_i(\tilde{\Gamma}(-\tau)) \exp(o(N)) | \exp(o(N)) = \int_0^\tau dt \tilde{h}_a(-t, \tilde{\Gamma}(-\tau)) \exp(o(N)) \quad (5.46) \]

where the third line is obtained by using an argument in section 4.5, and the forth line comes from the Liouville’s theorem.

Similarly, the weight on the time reversed trajectory segment \( W(\{\tilde{\Gamma}(t), \ -\tau \leq t \leq 0\}) \) is written as

\[ W(\{\tilde{\Gamma}(t), \ -\tau \leq t \leq 0\}) = \int_0^\tau dt \tilde{h}_a(t, \Gamma(0)) \exp(o(N)). \quad (5.47) \]

(See Eq. (5.57) for the definition of \( h_a(t, \Gamma(0)) \).

### 5.3. Reversibility paradox

Suppose that there is a trajectory segment \( \{\Gamma(t), \ 0 \leq t \leq \tau\} \) from an energy surface \( \Sigma_0 \) to \( \Sigma_1 \). Then, the time reversed one \( \{\tilde{\Gamma}(t), \ -\tau \leq t \leq 0\} \) goes from \( \Sigma_1 \) to \( \Sigma_0 \). One may wonder how this fact is compatible with thermodynamic irreversibility. The essentially same question was proposed by Roschmidt, and has been known as the reversibility paradox. A standard answer may be replying on the operational impossibility of the time reverse operation \( \Gamma \rightarrow \mathcal{R} \Gamma \). If we were allowed to operate the system by using the result of the observation of the trajectory, we could perform the time reverse operation. This consideration is related to the Maxwell’s demon’s problem. However, the time dependence of \( \alpha \) is given without any references of trajectories. Thus, in our problem, the time reverse operation cannot be realized by \( \alpha() \) and the Maxwell’s demon problem does not appear.

However, still the paradox is not resolved completely. In order to be compatible with thermodynamic irreversibility, there should be asymmetry between the trajectory segment \( \{\Gamma(t), \ 0 \leq t \leq \tau\} \) and the time-reversed one \( \{\tilde{\Gamma}(t), \ -\tau \leq t \leq 0\} \). The asymmetry cannot come from a purely mechanical consideration. We must consider the measure for the ensemble of the initial conditions of the time-reversed trajectory segment \( \{\tilde{\Gamma}(t), \ -\tau \leq t \leq 0\} \). This ensemble, \( \mathcal{Y}_r \), is defined as a \((2N-1)\)-dimensional set which satisfies

\[ \tilde{U}_{0,-\tau}(\mathcal{Y}_r) = \Sigma_0. \quad (5.48) \]
From the reversibility relation Eq. (5.5), we obtain
\[ \mathcal{Y}_\tau = \mathcal{R}\mathcal{U}_{\tau,0}(\Sigma_0). \]
(5.49)

Owing to the chaotic nature, \( \mathcal{Y}_\tau \) becomes a quite complicated set as \( \tau \) is large. Here, we describe the set \( \mathcal{Y}_\tau \) informally. We focus on the thermodynamic limit so that the structure of \( \mathcal{Y}_\tau \) is clearly seen.

Suppose that the most probable processes \( \Sigma_0 \rightarrow \Sigma_1 \) and \( \Sigma_1 \rightarrow \Sigma_0 \) are realized by the protocols of the parameter change \( \alpha() \) and \( \tilde{\alpha}() \), respectively. Then, from Eq. (5.48), \( \mathcal{Y}_\tau \cap \Sigma_1 \) becomes dominant in \( \Sigma_1 \) with respect to the microcanonical measure for \( \Sigma_1 \). On the other hand, from Eq. (5.49), \( \mathcal{Y}_\tau \cap \Sigma_1 \) becomes dominant in \( \mathcal{Y}_\tau \) with respect to the microcanonical measure for \( \Sigma_0 \). One may wonder that these two statements are apparently contradictory. However, we should note that the measures are different when we observe the set \( \mathcal{Y}_\tau \). Here, it is worthwhile noting that \( \mathcal{Y}_\tau \cap \Sigma_1 \) is not dominant in \( \Sigma_1 \) with respect to the microcanonical measure for \( \Sigma_1 \), when \( \Sigma_1 \neq \tilde{\Sigma}_1 \). Therefore, we can imagine that the set \( \mathcal{Y}_\tau \) has a fine structure in energy surfaces apart from \( \tilde{\Sigma}_1 \). In order to represent this heterogeneity quantitatively, we define a measure \( \bar{\mu} \) for the set \( \mathcal{Y}_\tau \) as

\[ \bar{\mu}(\Delta_e(\tilde{\Gamma}(-\tau)); \mathcal{Y}_\tau) = \lim_{\delta E \to 0} \frac{\mu_L(\Delta_e(\tilde{\Gamma}(-\tau)) \cap \mathcal{R}\mathcal{U}_{\tau,0}(\Sigma_0 \circ \delta E))}{\mu_L(\mathcal{R}\mathcal{U}_{\tau,0}(\Sigma_0 \circ \delta E))}, \]
(5.50)

where \( \mu_L \) denotes the 2\( N \)-dimensional Lebesgue measure, \( \Delta_e(\tilde{\Gamma}(-\tau)) \) is a small region with a size \( \epsilon \) including \( \tilde{\Gamma}(-\tau) \), and \( \Sigma_0 \circ \delta E \) represents a set of energy surfaces with width \( \delta E \). (See section 2.4.)

We then expect that \( \bar{\mu}(\Delta_e(\tilde{\Gamma}(-\tau)); \mathcal{Y}_\tau) \) for \( \tilde{\Gamma}(-\tau) \in \Sigma_1 \) is much larger than \( \bar{\mu}(\Delta_e(\tilde{\Gamma}(-\tau)); \mathcal{Y}_\tau) \) for \( \tilde{\Gamma}(-\tau) \in \Sigma_1 \).

5.4. Reversibility in probability

In spite of the asymmetry between the two sets \( \Sigma_0 \) and \( \mathcal{Y}_\tau \), from the reversibility of the time evolution, there is a one-to-one correspondence between a set of trajectory segments from \( \Sigma_0 \) to \( \mathcal{R}\mathcal{Y}_\tau \) and a set of time-reversed trajectory segments from \( \mathcal{Y}_\tau \) to \( \Sigma_0 \).

We now derive the reversibility relation coming from this correspondence. In Section 4.7, we discussed the weight on trajectory segments. The weight \( W(\{\Gamma(t), 0 \leq t \leq \tau\}) \) is a conditional probability finding trajectory segments remaining in a small tube around \( \tilde{\Gamma}(t), 0 \leq t \leq \tau \) when the initial condition is chosen in a small region \( \Delta_e(\tilde{\Gamma}(0)) \) around \( \tilde{\Gamma}(0) \). Then,

\[ \mu_{mc}(\Delta_e(\tilde{\Gamma}(0)); \Sigma_0)W(\{\Gamma(t), 0 \leq t \leq \tau\}) \]
(5.51)

is a probability finding a trajectory segment in a small tube around \( \{\Gamma(t), 0 \leq t \leq \tau\} \) of all trajectory segments from \( \Sigma_0 \) to \( \mathcal{R}\mathcal{Y}_\tau \). The probability, from the one-to-one correspondence mentioned above, should be equal to a probability finding a trajectory segment in a small tube around \( \{\tilde{\Gamma}(t), -\tau \leq t \leq 0\} \) of all trajectory segments from \( \mathcal{Y}_\tau \) to \( \Sigma_0 \). The latter probability is written as

\[ \bar{\mu}(\Delta_e(\tilde{\Gamma}(-\tau)); \mathcal{Y}_\tau)W(\{\tilde{\Gamma}(t), -\tau \leq t \leq 0\}). \]
(5.52)

Therefore, we obtain the relation

\[ \mu_{mc}(\Delta_e(\tilde{\Gamma}(0)); \Sigma_0)W(\{\Gamma(t), 0 \leq t \leq \tau\}) = \bar{\mu}(\Delta_e(\tilde{\Gamma}(-\tau)); \mathcal{Y}_\tau)W(\{\tilde{\Gamma}(t), -\tau \leq t \leq 0\}). \]
(5.53)

This relation will lead to an important equality related to thermodynamic irreversibility.

§6. Irreversible information loss

6.1. Definition

Let us define the irreversible information loss \( I \) as

\[ I(\tau, \Gamma(0)) = \log \frac{W(\{\tilde{\Gamma}(t), -\tau \leq t \leq 0\})}{W(\{\Gamma(t), 0 \leq t \leq \tau\})}. \]
(6.1)
where the right-hand side depends on \((\tau, \Gamma(0))\) because the trajectory is given by a solution to the deterministic evolution equation. Using Eqs. (5.39) and (5.47), we can write \(I\) as

\[
I(\tau, \Gamma(0)) = \int_0^\tau dt [h_a(t, \Gamma(0)) - \tilde{h}_a(-t, \tilde{\Gamma}(-\tau))] + o(N).
\]

The expression may represent the meaning of the term 'irreversible information loss'. Then, from the relation Eq. (5.53), we obtain

\[
\int_{\Upsilon} \mu(\Delta_{\epsilon}(\Gamma(-\tau)); \tau) = \int_{\Sigma_0} \mu_{\text{mc}}(\Delta_{\epsilon}(\Gamma(0))) \exp(-I).
\]

By the normalization condition of the probability, we have the equality

\[
\langle \exp(-I) \rangle_0 = 1,
\]

where \(\langle \cdot \rangle_0\) denotes the average by \(\mu_{\text{mc}}(d\Gamma; \Sigma_0)\). Using the Jensen’s inequality

\[
\langle \exp(-I) \rangle_0 \leq \exp(-\langle I \rangle_0),
\]

we obtain

\[
\langle I \rangle_0 \geq 0.
\]

This inequality suggests that the irreversible information loss \(I\) has a certain relation with thermodynamic irreversibility. One may find that the argument has some similarity with that by Jarzinski.

In order to discuss the convergence of \(I(\tau, \Gamma(0))\) for \(\tau \to \infty\), we evaluate the value of

\[
\lim_{\tau \to \infty} \frac{\partial I}{\partial \tau} = \lim_{\tau \to \infty} [h_a(\tau, \Gamma(0)) - \tilde{h}_a(-\tau, \tilde{\Gamma}(-\tau))].
\]

Since the value of \(\alpha\) is changed in a finite time interval, \(\xi(t, \xi(0); \Gamma(0))\) approaches to the unstable manifold around \(\Gamma(t)\) when \(t \gg \tau_f\). We thus obtain

\[
\lim_{\tau \to \infty} [h_a(\tau, \Gamma(0)) - \tilde{h}_a(-\tau, \tilde{\Gamma}(-\tau))] = \lim_{\tau \to \infty} [h(\Gamma(\tau)) - h(\tilde{\Gamma}(\tau))] = \frac{d}{dt} o(N),
\]

where we have used Eq. (5.22). We further assume that this convergence is so fast that the time integration becomes a finite value. Then, there exists a function \(\bar{I}\) such that

\[
\lim_{\tau \to \infty} \lim_{N \to \infty} \frac{1}{N} I(\tau, \Gamma(0)) = \bar{I}(\Gamma(0)).
\]

6.2. Most probable value

We define the most probable value of \(\bar{I}(\Gamma(0))\) based on the assumption of the large deviation property:

Let \(\Pi_I(\psi; \Sigma_0, \alpha())d\psi\) be a probability such that \(I(\tau, \Gamma(0))/N\) takes a value in \([\psi, \psi + d\psi]\) when the initial equilibrium state \(\Sigma_0\) and the protocol of the parameter change \(\alpha()\) are given. Then, \(\Pi_I\) is written in the form

\[
\Pi_I(\psi; \Sigma_0, \alpha()) \sim \exp(-N \phi_I(\psi; \Sigma_0, \alpha())),
\]

in the thermodynamic limit.

The probability density \(\Pi_I\) is induced from the microcanonical measure for the initial conditions on \(\Sigma_0\). The rate function \(\phi_I\) is a convex and non-negative function, and the most probable value \(\bar{I}\) satisfies

\[
\phi_I(\bar{I}; \Sigma_0, \alpha()) = 0.
\]
Here, Eq. (6-13) leads to the inequality
\[ \bar{I}_s \geq 0 \]
for an arbitrary most probable process.

We then try to find a relation between \( \bar{I}_s \) and \( \Delta S_B \). First, let us note that \( \langle I \rangle_0 \) is rewritten as

\[
\langle I \rangle_0 = -\int_{\Sigma_0} \mu_{mc}(\Delta_e(\Gamma(0)); \Sigma_0) \log \frac{\mu(\Delta_e(\tilde{\Gamma}(\tau)); \Sigma_{\tau})}{\mu_{mc}(\Delta_e(\Gamma(0)); \Sigma_0)},
\]

where we have used Eq. (5-53). We consider the thermodynamic limit in the expression Eq. (6-14), although the argument is not completely formalized yet.

When the most probable process \( \Sigma_0 \rightarrow \Sigma_1 \) is realized, \( \Upsilon_{\tau} \cap \Sigma_1 \) is dominant in \( \Upsilon_{\tau} \) with respect to the microcanonical measure on \( \Sigma_0 \). Also, from the mixing property, \( \Upsilon_{\tau} \cap \Sigma_1 \) may be identified with \( \Sigma_1 \) in a coarse graining description of the phase space. Thus, we can expect that \( \bar{\mu}(\Delta_e(\tilde{\Gamma}(\tau)); \Sigma_{\tau}) \) in Eq. (6-14) may be replaced by \( \mu_{mc}(\Delta_e(\tilde{\Gamma}(\tau)); \Sigma_1) \exp(o(N)) \), in an appropriate limit of small \( \epsilon \), large \( \tau \), and large \( N \). When this expectation is valid, we can rewrite Eq. (6-14) as

\[
\langle I \rangle_0 = -\int_{\Sigma_0} \mu_{mc}(\Delta_e(\Gamma(0)); \Sigma_0) \log \frac{\mu_{mc}(\Delta_e(\tilde{\Gamma}(\tau)); \Sigma_1)}{\mu_{mc}(\Delta_e(\Gamma(0)); \Sigma_0)} + o(N),
\]

\[
= -\int_{\Sigma_0} \mu_{mc}(\Delta_e(\Gamma(0)); \Sigma_0) \log \frac{|\Sigma_0|}{|\Sigma_1|} + o(N).
\]

Thus, we obtain

\[ I_s = \lim_{N \rightarrow \infty} \frac{1}{N} \log \frac{\Omega_1}{\Omega_0}, \]

\[ = \lim_{N \rightarrow \infty} \frac{1}{N} [S_B(\Sigma_1) - S_B(\Sigma_0)]. \]

This equality Eq. (6-17) shows that the value of \( \bar{I}_s \) is determined by initial and final states irrespective of details of the process \( \Sigma_0 \rightarrow \Sigma_1 \). Furthermore, from Eqs. (5-28) in Section 3.2, we can express \( \bar{I}_s \) in the form

\[
\bar{I}_s = \lim_{N \rightarrow \infty} \frac{1}{N} \log \frac{\Omega_1}{\Omega_0},
\]

\[ = \lim_{N \rightarrow \infty} \frac{1}{N} [S_B(\Sigma_1) - S_B(\Sigma_0)]. \]

That is, the most probable value of the irreversible information loss is equal to the change of the Boltzmann entropy per a unit degree. Also, the inequality Eq. (6-13) can be read as

\[ S_B(\Sigma_1) \geq S_B(\Sigma_0) + o(N) \]

for an arbitrary most probable process \( \Sigma_0 \rightarrow \Sigma_1 \). This implies that the Boltzmann entropy satisfies the entropy principle in thermodynamics.

### 6.3. Fluctuation theorem

Let us consider a probability \( \Pi_I(\psi; \Upsilon_{\tau}, \alpha()) \exp(-d\psi) \) such that the irreversible information loss \( \bar{I} \) takes a value within \([N\psi, N(\psi + d\psi)]\) when the measure of the initial conditions is assumed to be \( \bar{\mu} \) and the time-reversed protocol \( \alpha() \) is given. \( \Pi_I(\psi; \Upsilon_{\tau}, \alpha()) \exp(-d\psi) \) is written as

\[
\bar{I}(\psi; \Upsilon_{\tau}, \alpha()) \exp(-d\psi) = \int_{\Upsilon_{\tau}} \mu(\Delta_e(\tilde{\Gamma}(\tau)); \Upsilon_{\tau}) \exp(-d\psi),
\]

where \( \exp(*) \) takes the value 1 when the statement \( * \) is true. The right-hand side of this expression is rewritten in the following way.

\[
\int_{\Upsilon_{\tau}} \mu(\Delta_e(\tilde{\Gamma}(\tau)); \Upsilon_{\tau}) \exp(-d\psi) \leq \bar{I}(\tau, \Gamma(0))/N \leq \psi + d\psi,
\]

\[
= \exp(N\psi) \int_{\Sigma_0} \mu_{mc}(\Delta_e(\Gamma(0))) \exp(-d\psi) \leq \bar{I}(\tau, \Gamma(0))/N \leq \psi + d\psi,
\]

\[
= \exp(N\psi) \Pi_I(-\psi; \Sigma_0, \alpha()) \exp(-d\psi),
\]
where we have used Eq. (5.53) in order to obtain the second line. Therefore, we obtain

\[
\frac{\Pi_I(\psi; \Sigma_0, \alpha())}{\tilde{\Pi}_I(-\psi; \tilde{\Sigma}_\tau, \tilde{\alpha}())} = \exp(N\psi). \tag{6.25}
\]

This may be called the fluctuation theorem in Hamiltonian systems with a time-dependent parameter.

We could not derive a useful expression of Eq. (6.25) in the thermodynamic limit. We explain the reason. Suppose that the most probable process $\tilde{\Sigma}_1 \rightarrow * \Sigma_0$ is realized by the time-reversed protocol $\tilde{\alpha}()$. Then, the dominant region of $\Upsilon_{\tau}$ with respect to the measure $\tilde{\mu}$, which contributes $\Pi_I(\psi; \Upsilon_{\tau}, \tilde{\alpha}())$ much, is around the energy surface $\tilde{\Sigma}_1$. However, if $\Upsilon_{\tau}$ was replaced by $\tilde{\Sigma}_1$, $\psi$ in Eq. (6.25) could not be substituted by, for example, the most probable value $\bar{I}_s$ for $\Sigma_0 \rightarrow * \Sigma_1$. This loses the significance of Eq. (6.25).

When we are concerned with an infinitely small step process, we can derive the fluctuation-response relation from Eq. (6.25). In such a process, $\Upsilon_{\tau}$ may be replaced by $\Sigma_0$ at the lowest order approximation. Then, since $\Pi_I$ may be approximated by a Gaussian distribution for large $N$, we can write

\[
\log \tilde{\Pi}_I(-\psi; \Sigma_0, \tilde{\alpha}()) = -\frac{N(\psi + \bar{I}_s)^2}{2\sigma^2} + o(N), \tag{6.26}
\]

\[
\log \Pi_I(\psi; \Sigma_0, \alpha()) = -\frac{N(\psi - \bar{I}_s)^2}{2\sigma^2} + o(N). \tag{6.27}
\]

The fluctuation theorem Eq. (6.25) leads to

\[
-\frac{N(\psi - \bar{I}_s)^2}{2\sigma^2} + \frac{N(\psi + \bar{I}_s')^2}{2\sigma'^2} = N\psi + o(N). \tag{6.28}
\]

Since $\bar{I}_s$ and $\bar{I}'_s$ are infinitely small, Eq. (6.28) may be valid for arbitrary $\psi$ in a finite range including $\psi = 0$. Thus, we have

\[
\bar{I}'_s = \bar{I}_s, \tag{6.29}
\]

\[
\sigma'^2 = \sigma^2. \tag{6.30}
\]

Substituting these equalities into Eq. (6.28), we obtain

\[
NI_s = \frac{N}{2} \sigma'^2 = \frac{N^2}{2} \left\langle (\delta\psi)^2 \right\rangle \tag{6.31}
\]

\[
= \frac{1}{2} \left\langle (I - N\bar{I}_s)^2 \right\rangle. \tag{6.32}
\]

Comparing Eq. (6.33) with Eq. (3.14) in Section 3.4, we find that this result is consistent with Eq. (6.19).

§7. Excess information loss

At each point $\Gamma(t)$ in a trajectory segment, $\{\Gamma(t), 0 \leq t \leq \tau\}$, we can consider a Hamiltonian system defined on the energy surface $\Sigma(t)$ by virtually fixing the parameter value to $\alpha(t)$. Then, as discussed in Section 4.4, we can calculate the information loss rate, $h(\Gamma; \Sigma(t))$ at $\Gamma \in \Sigma(t)$ in this virtual Hamiltonian system. We define the excess information loss rate as

\[
h_{ex}(t, \Gamma(0)) = h_s(t, \Gamma(0)) - h(\Gamma(t); \Sigma(t)). \tag{7.1}
\]

\* We obtained the idea of the excess information loss from a paper by Oono and Paniconi, where they defined the excess heat in constructing steady state thermodynamics.
Further, the excess information loss $H_{\text{ex}}$ is defined as the time integration of $h_{\text{ex}}$

$$H_{\text{ex}}(\tau, \Gamma(0)) = \int_0^\tau d\tau h_{\text{ex}}(t, \Gamma(0)). \quad (7.2)$$

Similarly, the excess information loss rate at $\tilde{\Gamma}(-t)$ in the time-reversed trajectory is given by

$$\tilde{h}_{\text{ex}}(-t, \tilde{\Gamma}(-\tau)) = \tilde{h}_a(-t, \tilde{\Gamma}(-\tau)) - h(\tilde{\Gamma}(-t); \Sigma(t)), \quad (7.3)$$

where $\tilde{\Gamma}(-t) \in \Sigma(t)$, and the excess information loss in the time-reversed trajectory is written as

$$\tilde{H}_{\text{ex}}(\tau, \tilde{\Gamma}(-\tau)) = \int_0^\tau d\tau \tilde{h}_{\text{ex}}(-t, \tilde{\Gamma}(-\tau)). \quad (7.4)$$

Using these quantities, we rewrite the irreversible information loss $I$ as

$$I(\tau, \Gamma(0)) = \int_0^\tau dt [h_a(t, \Gamma(0)) - \tilde{h}_a(-t, \tilde{\Gamma}(-\tau))] + o(N), \quad (7.5)$$

$$= \int_0^\tau dt [h_{\text{ex}}(t, \Gamma(0)) - \tilde{h}_{\text{ex}}(-t, \tilde{\Gamma}(-\tau))] + o(N), \quad (7.6)$$

$$= H_{\text{ex}}(\tau, \Gamma(0)) - \tilde{H}_{\text{ex}}(\tau, \tilde{\Gamma}(-\tau)) + o(N), \quad (7.7)$$

where we have used the equality

$$h(\Gamma(t); \Sigma(t)) = h(\tilde{\Gamma}(-t); \Sigma(t)) + \frac{d}{dt}o(N). \quad (7.8)$$

(See Eq. (5.22).) Further, through the definition of $H_{\text{ex:rev}}$

$$H_{\text{ex:rev}}(\tau, \Gamma(0)) = \frac{1}{2} [H_{\text{ex}}(\tau, \Gamma(0)) + \tilde{H}_{\text{ex}}(\tau, \tilde{\Gamma}(-\tau))], \quad (7.9)$$

Eq. (7.7) becomes

$$\frac{1}{2}I(\tau, \Gamma(0)) = H_{\text{ex}}(\tau, \Gamma(0)) - \tilde{H}_{\text{ex}}(\tau, \tilde{\Gamma}(0)) + o(N). \quad (7.10)$$

In the viewpoint of numerical calculation, the excess information loss is a more tractable quantity than the irreversible information loss, because $H_{\text{ex}}(\tau, \Gamma(0))$ converges to a certain value $H_{\text{ex}}(\infty, \Gamma(0))$ when $\tau \to \infty$. This convergence can be expected from a fact that $h_{\text{ex}}(t, \Gamma(0))$ converges to 0 when $t - \tau f \to \infty$. Similarly, we expect that $H_{\text{ex}}(\tau, \tilde{\Gamma}(-\tau))$ converges to a certain value $H_{\text{ex}}(\infty, \tilde{\Gamma}(-\infty))$ when $\tau_i \to \infty$. (Note that $\tau \to \infty$ when $\tau_i \to \infty$.) Also, $H_{\text{ex:rev}}(\infty, \Gamma(0))$ is determined.

Let us consider the average over the initial conditions sampled from the microcanonical ensemble on the energy surface $\Sigma_0$. From Eq. (7.10), we have

$$\frac{1}{2} N\bar{I}_s = \langle H_{\text{ex}} \rangle_0 - \langle H_{\text{ex:rev}} \rangle_0 + o(N) \quad (7.11)$$

in the thermodynamic limit, where $\langle H_{\text{ex}} \rangle_0$ is the average of $H_{\text{ex}}(\infty, \Gamma(0))$. Since $H_{\text{ex}}(\infty, \Gamma(0))$ can be obtained numerically without referring the time-reversed trajectory, $\langle H_{\text{ex}} \rangle_0$ is a directly measurable quantity. Although $\langle H_{\text{ex:rev}} \rangle_0$ is not easily obtained numerically, this may be expected to have a certain relation to the quasi-static excess information loss $H_{\text{ex:qs}}$, which is defined as

$$H_{\text{ex:qs}} = \int_0^\infty dt \frac{d}{dt} \Phi(\Sigma(t)), \quad (7.12)$$

where the quantity $\Phi(\Sigma(t))d\alpha$ is the excess information loss calculated under the assumption that the equilibrium state is virtually realized at each time $t$ along the trajectory $\Gamma(t)$. (Recall a similar discussion below Eq. (3.31).) Notice that $H_{\text{ex:qs}}$ becomes the real excess information loss when the process is quasi-static.
We are going to discuss the relation between $H_{\text{ex:rev}}$ and $H_{\text{ex:qs}}$. We consider a step process realized by an infinitely small parameter change $\alpha \rightarrow \alpha + \Delta \alpha$ at $t = \tau_i$. Then, the quantity $\Phi(\Sigma_0)$ is given by

$$\langle H_{\text{ex}} \rangle_0 = \Phi(\Sigma_0) \Delta \alpha + O((\Delta \alpha)^2).$$

(7.13)

Also, using Eqs. (3.40) and (6.19), we obtain

$$\bar{I}_* = O((\Delta \alpha)^2).$$

(7.14)

Therefore, we find

$$\langle H_{\text{ex:rev}} \rangle_0 = \Phi(\Sigma_0) \Delta \alpha + O((\Delta \alpha)^2).$$

(7.15)

Since a quasi-static process can be realized by repeating an infinite number of infinitely small step processes, $\langle H_{\text{ex:rev}} \rangle_0$ for a quasi-static process $\Sigma_0$qs $\rightarrow \Sigma_1$ is written as

$$\langle H_{\text{ex:rev}} \rangle_0 = \int_{\alpha_0}^{\alpha_1} d\alpha \Phi(\Sigma(\alpha)),$$

(7.16)

where $\Sigma(\alpha)$ is the equilibrium state such that

$$\Sigma_0 = \Sigma(\alpha_0) \xrightarrow{\text{qs}} \Sigma(\alpha).$$

(7.17)

Then, Eq. (7.16) implies

$$\langle H_{\text{ex:rev}} \rangle_0 = \langle H_{\text{ex:qs}} \rangle_0.$$

(7.18)

Note however that the validity of Eq. (7.18) is ensured only for quasi-static processes. Nevertheless, we assume that Eq. (7.18) holds at least near quasi-static processes. Based on the assumption, the right-hand side of Eq. (7.17) is calculated numerically without referring time-reversed trajectories, and from Eqs. (6.19), (7.17) and (7.18), we obtain the expression

$$\frac{1}{2} \langle \Delta S_B \rangle_0 = \langle H_{\text{ex}} \rangle_0 - \langle H_{\text{ex:qs}} \rangle_0 + o(N).$$

(7.19)

7.1. Minimum principle

Applying the inequality Eq. (6.13) to the expression Eq. (7.11), we obtain

$$\langle H_{\text{ex}} \rangle_0 \geq \langle H_{\text{ex:rev}} \rangle_0 + o(N).$$

(7.20)

This inequality implies that the excess information loss must not be lower than its reversible part. Such a phrase reminds us the minimum work principle in thermodynamics with an isothermal environment, which states that the work done by external agents must not be lower than the quasi-static work. As discussed in the previous subsection, $H_{\text{ex:rev}}$ may be related to the quasi-static excess information loss. Therefore, the analogy with the minimum work principle may be expected more and Eq. (7.20) may be regarded as the minimum excess information loss principle. However, we do not yet understand the significance of the inequality Eq. (7.20). We expect that the analysis of subsystems may provide us a further insight for Eq. (7.20). This will be a future problem.

7.2. Expression of $\Phi$

In this subsection, we derive an expression of $\Phi$ in terms of Lyapunov vectors. Suppose that the value of $\alpha$ is changed instantaneously from $\alpha_0$ to $\alpha_0 + \Delta \alpha$ at time $t = 0$. The trajectory $\Gamma(\cdot)$ is not differentiable at $t = 0$. We consider the excess information loss for $\Gamma(\cdot)$

$$H_{\text{ex}}(\infty, \Gamma(0)) = \int_0^\infty dt [h_a(t; \Gamma(0)) - h(\Gamma(t); \Sigma_1)],$$

(7.21)

where $\Sigma_1$ is an energy surface after the parameter change.
Let \( \{ \xi_i^{(0)} \}, \ 1 \leq i \leq 2N \) be a set of Lyapunov vectors at \( \Gamma(0) \) in the energy surface \( \Sigma_0 \). We then define a set of vectors \( \{ a_i(t), \ 1 \leq i \leq 2N \} \) in the tangent space at \( \Gamma(t) \) as

\[
a_i(t) = T(t, 0; \Gamma(0)) \xi_i^{(0)},
\]

(7.22)

where \( T(t, 0; \Gamma(0)) \) is the linearized evolution map along the trajectory in the energy surface \( \Sigma_1 \). Note that \( a_i \) is not the Lyapunov vector at \( \Gamma(t) \), because \( \xi_i^{(0)} \) is not the Lyapunov vector in the energy surface \( \Sigma_1 \).

The \( i \)-th Lyapunov vector along the trajectory \( \{ \Gamma(t), \ 0 \leq t \leq \infty \} \) in the energy surface \( \Sigma_1 \) is denoted by \( \xi_i^{(1)}(\Gamma(t)) \). The expansion factor \( A_i(t, \Gamma(0)) \) satisfies

\[
T(t, 0; \Gamma(0)) \xi_i^{(1)}(\Gamma(0)) = A_i(t, \Gamma(0)) \xi_i^{(1)}(\Gamma(t)).
\]

(7.23)

Using \( a_i \) and \( A_i \), we can write Eq. (7.21) as

\[
H_{ex}(\infty, \Gamma(0)) = \lim_{t \to \infty} | \log | \bigwedge_{i=1}^{N_p} a_i(t) | - \sum_{i=1}^{N_p} \log A_i(t, \Gamma(0)) |.
\]

(7.24)

Let us evaluate the right-hand side of Eq. (7.24). We expand \( \xi_i^{(0)} \) by the set of Lyapunov vectors \( \{ \xi_i^{(1)}(\Gamma(0)), \ 1 \leq i \leq 2N \} \) in such a way that

\[
\xi_i^{(0)} = \sum_{j=1}^{2N} Q_{ij} \xi_j^{(1)}(\Gamma(0)).
\]

(7.25)

Here, the matrix \( Q \) is defined at \( \Gamma(0) \) and depends on \( \Delta \alpha \). Then, from Eqs. (7.22) and (7.25), \( a_i(t) \) is expanded in the form

\[
a_i(t) = \sum_{j=1}^{2N} Q_{ij} A_j(t, \Gamma(0)) \xi_j^{(1)}(\Gamma(t)).
\]

(7.26)

Using this expression, we write \( | \bigwedge_{i=1}^{N_p} a_i(t) | \) as

\[
| \bigwedge_{i=1}^{N_p} a_i(t) | \simeq \log \left| \sum_{(j_1, \ldots, j_{N_p})} \left[ \prod_{k=1}^{N_p} Q_{j_k} \right] \left[ \prod_{k=1}^{N_p} A_{j_k}(t, \Gamma(0)) \right] \left[ \bigwedge_{k=1}^{N_p} \xi_k^{(1)}(\Gamma(t)) \right] \right|
\]

(7.27)

where the index \( j_k \) varies from 1 to 2N. When \( t \) is sufficiently large, the contribution from the unstable directions becomes dominant. Thus, for sufficiently large \( t \), we derive

\[
\log | \bigwedge_{i=1}^{N_p} a_i(t) | \simeq \log \left| \sum_{j_1=1}^{N_p} \cdots \sum_{j_{N_p}=1}^{N_p} \text{sgn}(j_1, \ldots, j_{N_p}) \prod_{k=1}^{N_p} A_{j_k}(t, \Gamma(0)) \prod_{k=1}^{N_p} Q_{j_k} \xi_k^{(1)}(\Gamma(t)) \right|
\]

(7.28)

\[
\simeq \log \det_{+} Q + \sum_{i=1}^{N_p} \log A_i(t, \Gamma(0)),
\]

(7.29)

where

\[
\det_{+} Q = \sum_{j_1=1}^{N_p} \cdots \sum_{j_{N_p}=1}^{N_p} \text{sgn}(j_1, \ldots, j_{N_p}) Q_{j_1} \cdots Q_{j_{N_p}}.
\]

(7.30)
and we have used the normalization condition $\left| \bigwedge_{i=1}^{N_p} \xi^{(1)}_i(\Gamma(t)) \right| = 1$. Finally, substituting Eq. (7.30) to Eq. (7.24), we obtain

$$H_{\text{ex}}(\infty, \Gamma(0)) = \log \det Q.$$  

(7.32)

Therefore, from the definition of $\Phi(\Sigma_0)$, we have

$$\Phi(\Sigma_0) = \lim_{\Delta\alpha \to 0} \frac{(\log \det Q)_0}{\Delta\alpha}.$$  

(7.33)

This expression shows that $\Phi$ takes a non-zero value when the unstable manifold varies linearly for the infinitely small parameter change.

§8. Numerical experiments

Until now, we have developed the theoretical arguments. However, one may point out that these lack the mathematical rigorousness. We then present evidences by numerical experiments so as to confirm the validity of the theoretical arguments.

As a direct experimental test of our theory, we should check the relation between the irreversible information loss and the Boltzmann entropy. However, unfortunately, we do not yet complete this test, because it is hard to measure numerically the irreversible information loss. The reasons of this hardness are as follows.

First, the time-reversed trajectory is needed in calculation of $I(\tau, \Gamma(0))$. This fact causes a delicate problem: Suppose that we obtain numerically a trajectory segment $\{\Gamma(t), 0 \leq t \leq \tau\}$. Since the system is chaotic, this trajectory is not an approximation of the true trajectory starting from the initial condition $\Gamma(0)$. However, when a pseudo-orbit tracing property is valid in the system, there is a true trajectory which is closed to the trajectory segment obtained numerically. Then, when we integrate the time-reversed equations of motion with the initial condition $\tilde{\Gamma}(-\tau)$, the trajectory obtained numerically deviates from $\{\tilde{\Gamma}(t), -\tau \leq t \leq 0\}$ due to the orbital instability. Therefore, in order to obtain the time-reversed trajectory $\{\tilde{\Gamma}(t), -\tau \leq t \leq 0\}$, we must store the data of the original trajectory.

Second, even if we obtain numerically $I(\tau, \Gamma(0))$, it does not converge to a value for $\tau \to \infty$, because only the extensive part of $I(\tau, \Gamma(0))$ converges. Therefore, it is not easy to choose the value of $\tau$ in numerical calculation. In principle, we have only to choose large $N$ so that the arbitrariness becomes less. However, we need much more time to study the systems with larger $N$.

In this paper, instead of the irreversible information loss, we discuss numerically the excess information loss, with particularly focusing on Eq. (7.19). Since $H_{\text{ex}}(\tau, \Gamma(0))$ converges to $H_{\text{ex}}(\infty, \Gamma(0))$ when $\tau \to \infty$, the numerical calculation of the excess information loss may be simpler than that of the irreversible information loss. Also, the time-reversed trajectory is not needed in the calculation of $H_{\text{ex}}$.

8.1. Model

A system consisting of many molecules with short-range repulsive interaction may be the most realistic model to study thermodynamic irreversibility. However, since we are concerned with a universal aspect of irreversibility, the choice of the system does not matter. Simpler models may be better to us. That is the reason why we study numerically the Fermi-Pasta-Ulam (FPU) model. The Hamiltonian of the FPU model is given by

$$H(\{q_i, p_i\}; g) = \sum_{i=1}^{N} \left[ \frac{1}{2} p_i^2 + \frac{1}{2} (q_{i+1} - q_i)^2 + \frac{g}{4} (q_{i+1} - q_i)^4 \right],$$  

(8.1)

where the value of $g$ is changed in time. That is, $\alpha()$ in previous sections is identified to $g()$ in this section.
The evolution equations for \( \{q_i\}, \{p_i\} \) are written as
\[
\begin{align*}
\frac{dq_i}{dt} &= p_i, \\
\frac{dp_i}{dt} &= (q_{i+1} - q_i) + g(q_{i+1} - q_i)^3 - (q_i - q_{i-1}) - g(q_i - q_{i-1})^3.
\end{align*}
\] (8.2) (8.3)

We assume periodic boundary conditions, \( q_0 = q_N \) and \( q_{N+1} = q_1 \) in Eq. (8.3). Under the boundary conditions, \( \sum_i p_i \) is a conserved quantity. We assume that the value of \( \sum_i q_i \) is zero, for simplicity. Then, \( \sum_i q_i \) also becomes a conserved quantity. We assume that the value of \( \sum_i q_i \) is zero. In the remaining part of this section, the energy surface with the condition \( \sum_i p_i = \sum_i q_i = 0 \) is simply called the energy surface. We solve numerically Eqs. (8.2) and (8.3) by the 4-th order symplectic integrator method with a time step \( \delta t = 0.005 \). Since we are concerned with the thermodynamic limit, we check the \( N \) dependence of our conclusions.

8.2. Lyapunov analysis

In this subsection, we assume that \( g \) takes a constant value, say \( g_0 \). Let \( E_0 \) be the energy. When \( E_0 g_0 \) is sufficiently large, the system with large \( N \) exhibits high-dimensional chaos. As an example of such parameter value set, \( (E_0, g_0) = (1.0, 10.0) \) is assumed.

We first check the mixing property with respect to the micro-canonical measure by discussing a relaxation behavior. (See the last paragraph of Section 2.3.) Figure 1 shows an example how the average of \( A \) relaxes to the equilibrium value when the initial conditions are sampled from an artificial ensemble we assumed. As far as we checked, we observed a similar relaxation behavior to the same equilibrium value for different sets of the initial conditions. We thus conclude numerically that the system possesses the mixing property. Therefore, the ensemble of the initial conditions at \( t = 0 \) is regarded as the microcanonical ensemble with the energy \( E_0 \) when the ensemble is made by sufficiently long time evolution of phase space points sampled from a distribution absolutely continuous to the Lebesgue measure on the energy surface. Here, we remark that the relaxation curve includes an oscillatory component, while the envelop curve exhibits an exponential decreasing behavior. Both the period of the oscillation and the relaxation time seem to be larger for larger \( N \).

Fig. 1. Relaxation behavior of the ensemble average of \( A \). \( N = 20 \). The ensemble of initial conditions is made artificially with fixing \( E \) and \( A \) as \( E = 1 \) and \( A(0) = 0.01 \). (b) log \( |\langle A \rangle - A_{eq}| \) versus \( t \). \( A_{eq} \) is the equilibrium value determined by the graph (a). The dotted line shows \( |\langle A \rangle - A_{eq}| = \exp(-t/50)/100 \).

In order to demonstrate the chaotic nature quantitatively, we show the Lyapunov exponents in Fig. 2. Notice that there are two additional zero Lyapunov exponents because of the momentum conservation. That is, \( N_p = N - 2 \). The convergence of orthonormal frames is confirmed in the way described in Section 4.2. Figure 3 shows the time evolution of the average of the distance \( d(\mathcal{F}(t, \Gamma(0))e_i, \mathcal{F}(t, \Gamma(0))e'_i) \) over initial conditions, where \( i = 1, 2, N - 3 \) and \( N - 2 \). We see that the distance decreases to a computational noise level after \( t = 3000 \).
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Fig. 2. Lyapunov spectrum. $N = 20$.

Fig. 3. Convergence of a set of orthogonal unit vectors. $N = 20$.

8.3. Boltzmann entropy

The Boltzmann entropy $S_B(E, g)$ is calculated numerically in the following way: First, according to the adiabatic theorem, which was discussed in Section 3.1, the phase space volume enclosed by an energy surface is conserved along quasi-static processes. Therefore, the equality

$$\Omega(E, g) = \Omega(E_*, 0)$$

holds for the quasi-static process $(E, g) \xrightarrow{qs} (E_*, 0)$. Since the FPU model with $g = 0$ is reduced to the harmonic oscillator model, $\Omega(E_*, 0)$ is given by the volume of the $2N - 2$ dimensional sphere, and is calculated as

$$\Omega(E_*, 0) = cE_*^{N-1},$$

where $c$ does not depend on $E_*$. Thus, the Boltzmann entropy at $(E, g)$ can be evaluated as

$$S_B(E, g) = S_B(E_*, 0) = (N - 1) \log E_*,$$

where an additive constant with respect to $E_*$ is omitted.

In numerical experiments, a quasi-static process $(E_0, g_0) \xrightarrow{qs} (E_1, g_0 + \Delta g)$ is realized by the large $\tau$ limit of the protocol $g(t) = g_0 + \Delta gt/\tau$ for $0 \leq t \leq \tau$. In Fig. 4, the average and deviation of $E_1$ are plotted against $\tau$. We find that the deviation becomes smaller for larger $\tau$, and we may assume

* In our previous paper, the factor in the right-hand side was written as $N - 2$, not $N - 1$. This was a mistake.
that quasi-static processes are realized when \( \tau > 100 \). The equi-entropy curve through \( \Sigma_0 = (E_0, g_0) \) in Fig. 3 was obtained in this way. We express the curve by \( E = E_{qs}(g; \Sigma_0) \). Similarly, as shown in Fig. 4, we can draw equi-entropy curves in the \((E, g)\) space.

![Fig. 4. (a) Average value of final energy versus \( \tau \). (b) Deviation of values of final energy versus \( \tau \). \( N = 20 \) and \( \Delta g = -1.0 \).](image)

Fig. 4. (a) Average value of final energy versus \( \tau \). (b) Deviation of values of final energy versus \( \tau \). \( N = 20 \) and \( \Delta g = -1.0 \).

![Fig. 5. Equi-entropy curve through \((E_0, g_0)\) (solid curve) and other equi-entropy curves (dotted line).](image)

Fig. 5. Equi-entropy curve through \((E_0, g_0)\) (solid curve) and other equi-entropy curves (dotted line).

Now, we consider a step process realized by the instantaneous change of the value of \( g \), from \( g_0 \) to \( g_1 = g_0 + \Delta g \), at \( t = 0 \). Then, the energy after the switching becomes \( E_1 \), whose value depends on the choice of the initial condition. The entropy difference \( \Delta S_B \) is calculated by

\[
\Delta S_B = S_B(E_1, g_1) - S_B(E_0, g_0),
\]

with the formula Eq. (8.6). In Fig. 6, the average of the entropy difference over the initial conditions, \( \langle \Delta S_B \rangle_0 \), is plotted against \( \Delta g \). This graph shows that \( \langle \Delta S_B \rangle_0 \) is positive. Also, as shown in Fig. 7, the relative fluctuation of \( \Delta S_B \) becomes less as \( N \) is increased. This implies the existence of the large deviation property of \( \Delta S_B \).

8.4. Excess information loss

We show the result of numerical calculation of the excess information loss for the step processes \((E_0, g_0) \rightarrow (E_1, g_0 + \Delta g)\). In Fig. 8, \( H_{ex}(t, \Gamma(0)) \) for four choices of the initial condition \( \Gamma(0) \) are plotted against \( t \). One can see that \( H_{ex}(\infty, \Gamma(0)) \) is clearly defined. In Fig. 9, we show the average of \( H_{ex}(t, \Gamma(0)) \) over the initial conditions chosen from the microcanonical ensemble on the energy surface \( \Sigma_0 \). \( \langle H_{ex} \rangle_0 \) is given as the value at \( t = \infty \) in this graph.

In Fig. 10, \( \langle H_{ex} \rangle_0 \) is plotted against \( \Delta g \). From this graph, we can evaluate the value of \( \Phi(\Sigma_0) \)
by the equality
\[
\langle H_{\text{ex}} \rangle_0 = \Phi(\Sigma_0) \Delta g + o(\Delta g)
\]
for \(\Delta g \to 0\). In a similar way, in principle, we can calculate the value of \(\Phi(\Sigma)\) at each energy surface. In particular, \(H_{\text{ex};qs}\) at the step process is given by
\[
H_{\text{ex};qs} = \frac{1}{2}(\Phi(\Sigma_0) + \Phi(\Sigma_1)) \Delta g,
\]
where \(\Sigma_1 = (E_1, g_1)\) and recall Eq. (8.12) for the definition of \(H_{\text{ex};qs}\).
Fig. 9. Average value of $H_{ex}(t, \Gamma(0))$ versus $t$. $N = 20$ and $\Delta g = 20$.

Fig. 10. $\langle H_{ex} \rangle_0$ versus $\Delta g$. Square and filled circle symbols represent the data for $N = 5$ and $N = 20$, respectively. The different normalizations for the $N$ dependence are used in (a) and (b).

8.5. Main experiment

In order to check the validity of Eq. (7.19), we need to calculate $\langle H_{ex;qs} \rangle_0$, the average of $H_{ex;qs}$ over the initial conditions. This is written as

$$\langle H_{ex;qs} \rangle_0 = \frac{1}{2}(\Phi(\Sigma_0) + \langle \Phi(\Sigma_1) \rangle_0)\Delta g.$$  

However, this average cannot be calculated efficiently, because $\Sigma_1$ depends on the choice of the initial condition, and $\Phi(\Sigma_1)$ is evaluated from a graph indicating $\Delta g$ versus the average of $H_{ex}$ over initial conditions sampled from the microcanonical ensemble on $\Sigma_1$. We thus find out a way to avoid the calculation of $H_{ex;qs}$. We perform the reversed experiments in which the parameter $g$ is changed from $g_1$ to $g_0$ with the initial state $\Sigma'_0 = (E_{qs}(g_1; \Sigma_0), g_1)$. Suppose that the process $\Sigma'_0 \rightarrow \Sigma'_1$ is realized, where $\Sigma'_1$ depends on the choice of the initial condition on the energy surface $\Sigma'_0$. Then, we can calculate the Boltzmann entropy change $\Delta S_B$ and the excess information loss, $H'_{ex}$, for the process $\Sigma'_0 \rightarrow \Sigma'_1$. These satisfy the relation

$$\frac{1}{2} \langle \Delta S_B \rangle'_0 = \langle H'_{ex} \rangle'_0 - \langle H'_{ex;qs} \rangle'_0 + o(N),$$  

(8-11)

where $\langle \rangle'_0$ denotes the average over the initial conditions sampled from the microcanonical ensemble on the energy surface $\Sigma'_0$, and $H'_{ex;qs}$ denotes the quasi-static excess information loss for the step process $\Sigma'_0 \rightarrow \Sigma'_1$. Here, we can prove the estimation

$$\langle H_{ex;qs} \rangle_0 + \langle H'_{ex;qs} \rangle'_0 = o((\Delta g)^2).$$  

(8-12)
(proof)

From the definition of $H_{ex:qs}$, we have

$$
\langle H'_{ex:qs} \rangle'_0 = -\frac{1}{2}(\Phi(\Sigma'_0) + \langle \Phi(\Sigma'_1) \rangle'_0)\Delta g.
$$

(8.13)

Using this equation and Eq. (8.9), we obtain

$$
\langle H_{ex:qs} \rangle_0 + \langle H'_{ex:qs} \rangle'_0 = \frac{1}{2}(\Phi(\Sigma_0) + \langle \Phi(\Sigma_1) \rangle_0)\Delta g.
$$

(8.14)

$$
-\frac{1}{2}(\Phi(\Sigma'_0) + \langle \Phi(\Sigma'_1) \rangle'_0)\Delta g.
$$

(8.15)

Recalling the energy change for step processes, we expect

$$
\Sigma'_0 - \Sigma_1 \sim O((\Delta g)^2),
$$

(8.16)

$$
\Sigma_0 - \Sigma'_1 \sim O((\Delta g)^2).
$$

(8.17)

Substitution these estimation to Eq. (8.15) leads to Eq. (8.12).

Finally, from Eqs. (7.19), (8.11) and (8.12), we obtain the equality

$$
\frac{1}{2}(\langle \Delta S_B \rangle_0 + \langle \Delta S_B \rangle'_0) = \langle H_{ex} \rangle_0 + \langle H'_{ex} \rangle'_0 + o(N, (\Delta g)^2).
$$

(8.18)

This relation can be checked numerically. As shown in Fig. 11, Eq. (8.18) seems valid, and therefore, our theoretical arguments turn out to be consistent.

![Fig. 11. $\langle H_{ex} \rangle_0 + \langle H'_{ex} \rangle'_0$ versus $\langle \Delta S_B \rangle_0 + \langle \Delta S_B \rangle'_0$. Square and filled circle symbols represent the data for $N = 5$ and $N = 20$, respectively. The sold line shows $\langle H_{ex} \rangle_0 + \langle H'_{ex} \rangle'_0 = 1/2[\langle \Delta S_B \rangle_0 + \langle \Delta S_B \rangle'_0]$.](image)

§9. concluding remark

The essence of thermodynamic irreversibility is described by the entropy principle. Therefore, when one discusses thermodynamic irreversibility from dynamical systems, the purpose is to find a state variable satisfying the entropy principle. Our arguments stand on this natural viewpoint. In this paper, we have found that the irreversible information loss leads to the state variable which satisfies the entropy principle.

We expect that our theory may be extended so as to apply to other dynamical systems without Hamiltonian. For example, in dissipative systems driven by external forces, a steady state is realized. The fluctuation properties have been discussed extensively. However, an attempt of the construction
of state theory seems scarcely. Although Oono and Paniconi have proposed an operational way to construct a state variable in steady state thermodynamics, its validity is not confirmed. We will attempt to construct non-equilibrium thermodynamic functions from dynamical system models by studying fluctuation properties.

Much variety of nonlinear dynamics have been known in the context of fluid systems, granular systems, chemical reaction systems, and biological systems. In these systems, the notion of entropy is not self-evident, and hardly connected to that in thermodynamics. Even in such systems, it may be important to characterize a state of the systems in terms of state functions representing a relation between states. In particular, one of the most serious questions in science may be the boundary of the living state. One may ask why we cannot restore the living state when a life is dead. This is not the problem of thermodynamic irreversibility, but there is a sort of irreversibility in a biological world. However, the question is too general to be discussed scientifically. We should argue more restricted phenomena related to this question. The determination of cell types in cell differentiation processes may be a good candidate. As already studied by Kaneko et al. from the dynamical system viewpoint, a cell society may be modeled by chemical networks with the variable number of cells. In these studies, Kaneko et al. have found that the rule of the determination of cell types emerges. We expect that the rule might be formalized by state space theory which shares common features with thermodynamics. As developed in our theory concerning thermodynamic irreversibility, we hope to find a quantity representing a sort of relation associated with biological irreversibility.

Acknowledgments

The authors express special thanks to Y. Oono for thoughtful ideas on thermodynamics and enlightening discussions. They acknowledge K. Sekimoto, H. Tasaki and S. Takesue for fruitful discussions on thermodynamic irreversibility; N. Nakagawa for helpful discussions on dynamical systems; M. Sano and T. Hatano for discussions on the fluctuation theorem; T. Chawanya, N. Ito and K. Sato for useful comments on the study; K. Kaneko for stimulating discussions on the future perspective; P. Gaspard and J. R. Dorfmann for their lectures at Hayama. One of the authors (T.S.K.) thanks RIKEN for their hospitality and acknowledges the support from JSPS Research Fellow.

Appendix

We summarize basic properties of the $k$-dimensional volume element and $k$-fold exterior product of vectors. Consider a $k$-dimensional surface in the $n$-dimensional Euclid space $\mathbb{R}^n$. The surface can be decomposed into a set of sufficiently small pieces of $k$-dimensional parallelalids. A $k$-dimensional parallelaid including a point $x \in \mathbb{R}^n$ is identified to that in a tangent space at $x \in \mathbb{R}^n$.

The $k$-dimensional volume of the projection of the parallelaid to a space spanned by $\{e_i, 1 \leq j \leq k\}$ is denoted by $\omega_{i_1i_2\cdots i_k} dx_{i_1} \cdots dx_{i_k}$, where $dx_{i_1} \cdots dx_{i_k}$ is a $k$-dimensional volume measure in the space spanned by $\{e_i, 1 \leq j \leq k\}$. A set $\{\omega_{i_1\cdots i_k}\}$ is called the $k$-dimensional volume element.

Let us write the $k$-dimensional volume element in a coordinate-free form. We consider the parallelaid $B$ made by a set of vectors $\{b_i, 1 \leq i \leq k\}$. We then define the $k$-fold exterior product $b_1 \wedge \cdots \wedge b_k$ as a map from a $k$-dimensional parallelaid to its $k$-dimensional volume of the projection to $B$. Explicitly, for a $k$-dimensional parallelaid made by a set of vectors $\{a_i, 1 \leq i \leq k\}$, the action of the map $b_1 \wedge \cdots \wedge b_k$ is defined as

$$b_1 \wedge \cdots \wedge b_k \cdot (a_1, \cdots a_k) = \det G,$$

where $G_{ij} = (b_i, a_j)$. We write $b_1 \wedge \cdots \wedge b_k$ as $\wedge_{i=1}^k b_i$, when the order of the vectors is uniquely guessed.

Then, we can find an exterior product $\wedge_{i=1}^k \omega_{i}$ such that

$$\omega_{i_1\cdots i_k} = \wedge_{i=1}^k \omega_{i} \cdot (e_{i_1}, \cdots e_{i_k}).$$
Since the exterior product is uniquely determined, $k$-dimensional volume element is identified with the $k$-fold exterior product. (A set of vectors $\{\omega_i, 1 \leq i \leq k\}$ is not uniquely determined.)

The $k$-fold exterior product $\wedge_{i=1}^{k} b_i$ has two important properties, multi-linearity and skew-symmetry. The multi-linearity is the relation

$$b_1 \wedge \cdots \wedge (c_i b_i + c_i' b'_i) \wedge \cdots \wedge b_k = c_i b_1 \wedge \cdots \wedge b_i \wedge \cdots \wedge b_k \tag{A.3}$$

$$+ c_i' b_1 \wedge \cdots \wedge b'_i \wedge \cdots \wedge b_k \tag{A.4}$$

for arbitrary $i$, where $c_i$ and $c_i'$ are numbers, and the skew-symmetry is

$$\wedge_{i=1}^{k} b_i = \text{sgn}(i_1, \ldots, i_k) \wedge_{i=1}^{k} b_i, \tag{A.5}$$

where $\text{sgn}(i_1, \ldots, i_k)$ takes a value 1 when the permutation $(1, \ldots, k) \to (i_1, \ldots, i_k)$ is generated by an even number of exchanges, otherwise it takes a value -1.

Using the two properties, we can prove

$$\wedge_{i=1}^{k} \sum_{j=1}^{k} G_{ij} b_j = \det G \wedge_{i=1}^{k} b_i. \tag{A.6}$$

(proof)

$$\wedge_{i=1}^{k} \sum_{j=1}^{k} G_{ij} b_j = \sum_{(j_1, \ldots, j_k)} G_{1j_1} b_{j_1} \wedge \cdots \wedge G_{kj_k} b_{j_k} \tag{A.7}$$

$$= \sum_{(j_1, \ldots, j_k)} G_{1j_1} \cdots G_{kj_k} b_{j_1} \wedge \cdots \wedge b_{j_k} \tag{A.8}$$

$$= \sum_{(j_1, \ldots, j_k)} \text{sgn}(j_1 \cdots j_k) G_{1j_1} \cdots G_{kj_k} b_{j_1} \wedge \cdots \wedge b_{j_k} \tag{A.9}$$

$$= \det G b_1 \wedge \cdots \wedge b_k. \tag{A.10}$$

The $k$-dimensional volume of the parallelipiped $B$ is calculated as $\sqrt{\text{det}B}$, where $B_{ij} = (b_i, b_j)$. We represent it by $| \wedge_{i=1}^{k} b_i |$.

(proof)

We can find a set of orthogonal unit vectors $\{u_i, 1 \leq i \leq k\}$ which generate the vector space spanned by $\{b_i, 1 \leq i \leq k\}$. (One may construct $\{u_i, 1 \leq i \leq k\}$ by employing the Gram-Schmidt procedure.) Then, the $k$-dimensional volume of $B$ is given by

$$| \wedge_{i=1}^{k} b_i | = | \wedge_{i=1}^{k} b_i \cdot (u_1, \ldots, u_k) |. \tag{A.11}$$

Since $b_i$ can be expanded in the form

$$b_i = \sum_{j=1}^{k} G_{ij} u_j, \tag{A.12}$$

we obtain

$$\wedge_{i=1}^{k} b_i = \det G \wedge_{i=1}^{k} u_i, \tag{A.13}$$

where we have used Eq. (A.6). Using the identity

$$\wedge_{i=1}^{k} u_i \cdot (u_1, \ldots, u_k) = 1, \tag{A.14}$$

we can rewrite Eq. (A.11) as

$$| \wedge_{i=1}^{k} b_i | = |\det G|. \tag{A.15}$$
On the other hand, since

\[(b_i, b_j) = \sum_{lm} G_{il} G_{jm} (u_l, u_m), \quad (A.16)\]

\[= \sum_l G_{il} G_{jl}, \quad (A.17)\]

\[= (GG^\dagger)_{ij}, \quad (A.18)\]

we have

\[B = GG^\dagger. \quad (A.19)\]

Therefore, the equality

\[\det B = (\det G)^2 \quad (A.20)\]

holds. Substituting this equality into Eq. (A.13), we obtain

\[|\wedge_{i=1}^k b_i| = \sqrt{\det B}. \quad (A.21)\]

(q.e.d)

Further, for arbitrary \(l\) such that \(1 \leq l \leq k\), the inequality

\[|b_1 \wedge \cdots \wedge b_k| \leq |b_1 \wedge \cdots \wedge b_l| |b_{l+1} \wedge \cdots \wedge b_k| \quad (A.22)\]

holds. This makes us possible to define ‘angle’ \(\phi\) between \(b_1 \wedge \cdots \wedge b_l\) and \(b_{l+1} \wedge \cdots \wedge b_k\) in such a way that

\[|b_1 \wedge \cdots \wedge b_l| = |b_1 \wedge \cdots \wedge b_l| |b_{l+1} \wedge \cdots \wedge b_k| \sin \phi. \quad (A.23)\]

(proof)

As seen in the previous proof, there exist two sets of orthogonal unit vectors \(\{u_i, \ 1 \leq i \leq l\}\) and \(\{u'_i, \ l + 1 \leq i \leq k\}\) such that

\[b_1 \wedge \cdots \wedge b_l = |b_1 \wedge \cdots \wedge b_l| u_1 \wedge \cdots \wedge u_l, \quad (A.24)\]

\[b_{l+1} \wedge \cdots \wedge b_k = |b_{l+1} \wedge \cdots \wedge b_k| u'_{l+1} \wedge \cdots \wedge u'_k, \quad (A.25)\]

where notice that \(u_i\) is not orthogonal to \(u'_j\). Then, we have

\[|b_1 \wedge \cdots \wedge b_k| = |b_1 \wedge \cdots \wedge b_l| |b_{l+1} \wedge \cdots \wedge b_k| |u_1 \wedge \cdots \wedge u_l \wedge u'_{l+1} \wedge \cdots \wedge u'_k|. \quad (A.26)\]

Now, by using the Gram-Schmidt orthogonalization, we define a new set of vectors \(\{u_j, \ l + 1 \leq j \leq k\}\) as

\[u_j = \frac{u'_j - \sum_{m=1}^{j-1} (u'_j, u_m) u_m}{s_j} \quad (A.27)\]

with

\[s_j = |u'_j - \sum_{m=1}^{j-1} (u'_j, u_m) u_m|. \quad (A.28)\]

Here, from the equality

\[|u'_j - \sum_{m=1}^{j-1} (u'_j, u_m) u_m|^2 + |\sum_{m=1}^{j-1} (u'_j, u_m) u_m|^2 = 1, \quad (A.29)\]

we find

\[0 \leq s_j \leq 1. \quad (A.30)\]
Then, from

\[ u_j' = s_j u_j + \sum_{m=1}^{j-1} (u_j', u_m) u_m, \]

we derive

\[ |u_1 \wedge \cdots \wedge u_k \wedge u_{k+1}' \wedge \cdots \wedge u_k'| = s_{l+1} \cdots s_k. \]

(A.32)

Substituting Eq. (A.32) into Eq. (A.26), we finally obtain

\[ |b_1 \wedge \cdots \wedge b_k| = |b_1 \wedge \cdots \wedge b_l| |b_{l+1} \wedge \cdots \wedge b_k| s_{l+1} \cdots s_k \]

(A.33)

\[ \leq |b_1 \wedge \cdots \wedge b_l| |b_{l+1} \wedge \cdots \wedge b_k|. \]

(A.34)

(q.e.d)

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