A non-equilibrium equality in Hamiltonian chaos

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We numerically study a billiard system with a time-dependent force, and our results suggest the existence of a limitation on possible transitions between steady states in Hamiltonian chaos, in analogy to the limitation on transitions between equilibrium states described by the second law of thermodynamics. This limitation is expressed in terms of irreversible information loss, which is defined for each trajectory through Lyapunov analysis. As a key step in the study, we demonstrate a non-equilibrium equality which means that the average of the inverse exponential of the irreversible information loss is unity, where the average is taken over initial conditions sampled from the microcanonical ensemble.

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The second law of thermodynamics is a formalization of a fundamental limitation on possible transitions among equilibrium states [1]. Although the validity of the second law has been confirmed conclusively without exception for more than a century, there yet exists no clear understanding of how this limitation emerges from purely Hamiltonian systems.

When the dynamical system in question possesses a mixing property, time correlations of dynamical variables decay. This decay characterizes the directional evolution in dynamical systems. For this reason, it may be natural to believe that the chaotic behavior of a system is related to the limitation on possible transitions between its steady states. However, as far as we know, such a description has never been formulated explicitly.

In this Letter, we study non-steady behavior of Hamiltonian chaos resulting from a change in the value of a parameter during a finite time interval. We define a quantity $I$, called the ‘irreversible information loss’, for each trajectory, and demonstrate that it satisfies the non-equilibrium equality

$$\langle \exp(-I) \rangle_{mc} = 1,$$

(1)

where $\langle \cdot \rangle_{mc}$ denotes the average over initial conditions sampled from the microcanonical ensemble on an energy surface specified initially. Through the Jensen inequality, $\langle \exp(-I) \rangle_{mc} \geq \exp(-\langle I \rangle_{mc})$, the inequality

$$\langle I \rangle_{mc} \geq 0$$

(2)

is derived. This may be regarded as a representation of the limitation on possible transitions.

Our search for a non-equilibrium equality of the form (1) for Hamiltonian chaos was initially motivated by its obvious relation to the Jarzynski equality [2,3]

$$\langle \exp(-\beta(W - \Delta F)) \rangle_c = 1,$$

(3)

where $W$ is the work done by an external agent, $\Delta F$ is the free energy increment for a state transition, and $\langle \cdot \rangle_c$ is the average over all possible histories, each of whose weight is determined by the probabilities of equilibrium fluctuations of the system in an isothermal environment with inverse temperature $\beta$. We note that the minimum work principle $\langle W \rangle_c \geq \Delta F$ can be derived as the result of (3). Considering the similarity of (3) and (1), it is natural to call (1) a Jarzynski-type equality in Hamiltonian chaos.

Although the analysis we give here can be applied to a fairly general class of Hamiltonian systems, we focus on a billiard system with a time-dependent external force. Here, each phase space point $\Gamma$ is specified by the canonical coordinates $(q_1, q_2, p_1, p_2)$, and the Hamiltonian we study is given by

$$H(\{q_1, p_1\}; f) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{d}(r(q_1)^2 + q_2^2)^{d/2} + fq_1,$$

(4)

with

$$r(q_1) = \theta(q_1)\max(q_1 - a, 0) + \theta(-q_1)\min(q_1 + a, 0),$$

(5)

where $\theta$ is the Heaviside step function. The quantity $f$ in (4) is an external force and the potential represents a soft interaction with a stadium-shape wall. In this Letter, we set $(d, a) = (8.0, 0.5)$. We numerically solved the evolution equations.
\[
\frac{dq_i}{dt} = p_i, \quad (6)
\]
\[
\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} \quad (7)
\]
by employing the 4-th order symplectic integrator method with a time step \( \delta t = 10^{-3} \).

We begin our discussion by describing the basic properties of the system in the case of a time-independent force, say \( f = f_0 \). Then, the energy is a constant, say \( E_0 \). As an example, we consider the case in which \( E_0 = 1.0 \) and \( f_0 = 0.0 \). Our numerical results for this system lead us to conclude that it does indeed possesses the mixing property with respect to the microcanonical measure. We thus assume that a continuous distribution of initial conditions on an energy surface evolves into the microcanonical ensemble in the weak sense when the system is left for a sufficiently long time.

The chaotic nature of the system is explored by applying a linear analysis (the 'Lyapunov analysis') to trajectories. Through the numerical integration of the linearized equations of motion corresponding to (6) and (7),

\[
\frac{d\delta q_i}{dt} = \delta p_i, \quad (8)
\]
\[
\frac{d\delta p_i}{dt} = -\sum_j \frac{\partial^2 H}{\partial q_i \partial q_j} \delta q_j, \quad (9)
\]
we obtained a tangent evolution map from time \( s \) to \( t \), \( T(t, s) \).

To make the discussion more concrete, we choose a specific reference time \( t_* \) and consider a set of four orthogonal unit vectors \( \{e_i(t_*)\} \) defined in the tangent space at the phase space point \( \Gamma(t_*) \) at time \( t_* \). Then, the vector \( e_i(t_*) \) evolves to \( T(t, t_*)e_i(t_*) \) in the tangent space at the phase space point \( \Gamma(t) \). By employing the Gram-Schmidt procedure \( T(t, t_*)e_i(t_*) \) (where \( t \geq t_* \)) can be expressed as

\[
T(t, t_*)e_i(t_*) = \sum_{j=1}^{4} e_j(t)L_{ji}(t, t_*), \quad (10)
\]

where \( L_{ij} \) is the \((i, j)\) element of an upper triangular matrix whose diagonal elements are positive, and \( \{e_i(t)\} \) is the set of four orthogonal unit vectors defined in the tangent space at the phase space point \( \Gamma(t) \). The \( n \)-th Lyapunov exponent \( \lambda_i \) is calculated as the long time average of the quantity \( \lambda_i(t) \) given by

\[
\lambda_i(t) = \frac{d}{dt} \log L_{ii}(t, t_*). \quad (11)
\]

Although the vector \( e_i(t) \) and the quantity \( \lambda_i(t) \) depend on the choice of the set \( \{e_i(t_*)\} \), the value of \( \lambda_i \) is independent of this choice for the system in question, and we have \( \lambda_1 = -\lambda_4 > 0 \) and \( \lambda_2 = \lambda_3 = 0 \).

There is a special vector \( e_1^{(S)}(\Gamma(t); f_0) \) at the point \( \Gamma(t) \), which is defined as

\[
e_1^{(S)}(\Gamma(t); f_0) = \lim_{t \to -\infty} e_1(t). \quad (12)
\]

In our numerical experiments, we insure that \( e_1^{(S)}(\Gamma(t); f_0) \) is represented by \( e_1(t) \) by choosing the value of \( t_* \) so that \( t - t_* \) is sufficiently large for the condition

\[
|1 - (e_1(t), e_1^{(S)}(t)^2)| \leq \epsilon \quad (13)
\]
to be satisfied for two vectors \( e_1(t_*) \) and \( e_1^{(S)}(t_*) \) chosen randomly, where \( \epsilon \) is arbitrarily chosen to be \( 10^{-6} \). The vector \( e_1^{(S)}(\Gamma(t); f_0) \) corresponds to the most unstable direction and is called the 'first Lyapunov vector' at the point \( \Gamma(t) \). Using this vector, we can define the first local expansion ratio as

\[
\lambda_1^{(S)}(\Gamma(t); f_0) = \frac{d}{dt} \log L_{11}^{(S)}(t, t_*), \quad (14)
\]
where \( L_{11}^{(S)}(t, s) \) is the magnitude of the vector \( T(t, t_*)e_1^{(S)}(\Gamma(t_*); f_0) \).

One may expect that \( \lambda_2^{(S)}(\Gamma(t); f_0) \) and \( \lambda_3^{(S)}(\Gamma(t); f_0) \) can be defined similarly to \( \lambda_1^{(S)}(\Gamma(t); f_0) \) and \( \lambda_1^{(S)}(\Gamma(t); f_0) \). However, numerically, the convergence condition in this case, taking a form similar to (13), is difficult to realize.
We thus added an artificial, small damping term $-\eta \delta \rho_i$ to $\tilde{\Gamma}$ in order to obtain $e_2^{(S)}(\Gamma(t); f_0)$. We expect the value obtained for $e_2^{(S)}(\Gamma(t); f_0)$ in this manner to be well-defined in the limit $\eta \to 0_+$ after first taking $t_\ast \to -\infty$. We call the subspace spanned by $e_1^{(S)}(\Gamma(t); f_0)$ and $e_2^{(S)}(\Gamma(t); f_0)$ the ‘semi-unstable space’.

Next, we consider the system with a time-dependent force. We consider a function $f(t)$ that changes from $f_0$ to $f_1$ only during a finite time interval $[t_0, t_1]$. The initial conditions at $t = \tau_-$ $(< t_0)$ are sampled from the microcanonical ensemble on an energy surface with energy $E_0$.

The Lyapunov analysis for the time-dependent system is developed in the following way. First, using the Gram-Schmidt decomposition of the linearized evolution map $T(t, s)$, the time evolution of a set of orthogonal unit vectors is determined. However, the Lyapunov vector $e_i(t; f_0)$ does not have meaning for $t > t_0$. Instead, we define the ‘forward Lyapunov vector’ $e_i^{(F)}(t)$ as the unit vector at time $t$ obtained from $e_i(t; f_0)$ under the Gram-Schmidt procedure, and the ‘backward Lyapunov vector’ $e_i^{(B)}(t)$ as the unit vector from which $e_i(t; f_1)$ is obtained under the Gram-Schmidt procedure, where $t_1 < \tau_+$. Since $L_{ii}^{(F)}(t, \tau_-)$ and $L_{ii}^{(B)}(\tau_+, t)$ are determined simultaneously with $e_i^{(F)}(t)$ and $e_i^{(B)}(t)$ through these Gram-Schmidt procedures, we define the forward local expansion ratio $\lambda_i^{(F)}(t)$ as

$$\lambda_i^{(F)}(t) = \frac{d}{dt} \log L_{ii}^{(F)}(t, \tau_-),$$

and the backward local expansion ratio $\lambda_i^{(B)}(t)$ as

$$\lambda_i^{(B)}(t) = \frac{d}{dt} \log L_{ii}^{(B)}(\tau_+, t).$$

(16)

When the force $f$ is time-independent (say $f_0$), three quantities $\lambda_i^{(F)}(t)$, $\lambda_i^{(B)}(t)$ and $\lambda_i^{(S)}(\Gamma(t); f_0)$ are identical. This leads us to conjecture that the difference between $\lambda_i^{(F)}(t)$ and $\lambda_i^{(B)}(t)$ provides a useful characterization of phenomena exhibited uniquely by time-dependent systems. Also, the long time average of $\lambda_i^{(S)}(\Gamma(t); f_0)$ is known to be equal to the information loss rate. With these in mind, we define the irreversible information loss $I$ as

$$I = \lim_{\eta \to 0_+} \int_{\tau_-}^{\tau_+} dt \sum_{i=1}^{2} \left[ \lambda_i^{(F)}(t) - \lambda_i^{(B)}(t) \right],$$

(17)

where we remark that the sum is taken over indices corresponding to the semi-unstable space, not unstable space.

Now, we present numerical results which indicate that the non-equilibrium equality (1) holds for the irreversible case. Instead, we define the irreversible information loss $I$ defined by $I$. We first note that $e_i^{(B)}(t)$ cannot be calculated directly, because the backward evolution of the semi-unstable space is not numerically stable. Thus, in order to be able to apply the type of analysis we discuss here to the general situation, we need to devise some more sophisticated algorithm to calculate $e_i^{(B)}(t)$. In this Letter, however, we focus on the simplest case in which $f$ is changed from $f_0$ to $f_1$ instantaneously at $t = t_0$. In this case, when $t \geq t_0$, $e_i^{(B)}(t)$ and $\lambda_i^{(B)}(t)$ are equal to $e_i^{(S)}(\Gamma(t); f_1)$ and $\lambda_i^{(S)}(\Gamma(t); f_1)$, respectively. That is, the integration over the region $t_0 \leq t \leq t_+ 1$ in $I$ can be done numerically. The other part of integration can be evaluated with the aid of the time-reversed trajectory $\{\tilde{\Gamma}(t)\}_{t=\tau_-}$, which is the solution to the Hamiltonian equation with the time-reversed external force, $\{\tilde{f}(t)\}_{t=\tau_-}$, and with the initial condition $\tilde{\Gamma}(\tau_-) = R\Gamma(\tau_+)$, where $R$ is the operator that changes the sign of the momentum. We can carry out Lyapunov analysis for the time-reversed trajectory, and we express all quantities obtained in this analysis by simply adding a tilde to the corresponding quantities in the normal Lyapunov analysis. From the reversibility of the Hamiltonian equations, the integration over the region $\tau_- \leq t \leq t_0$ in $I$ turns out to be equal to

$$\int_{t_0}^{\tau_-} dt \sum_{i=1}^{2} \left[ \tilde{\lambda}_i^{(F)}(t) - \tilde{\lambda}_i^{(B)}(t) \right] + \log \frac{\sin \theta^{(B)}(t_0)}{\sin \theta^{(F)}(t_0)},$$

(18)

where $\sin \theta^{(F)}(t_0)$ is the four dimensional volume spanned by the vectors $e_i^{(F)}(t_0)$ and $R e_i^{(F)}(t_0)$ ($i = 1, 2$), and $\sin \theta^{(B)}(t_0)$ is defined similarly. The quantity $I$ can be calculated by using the forward evolution of the semi-unstable space, because $\tilde{\lambda}_i^{(B)}(t)$ and $\tilde{e}_i^{(B)}(t)$ are identical to $\lambda_i^{(S)}(\Gamma(-t); f_0)$ and $e_i^{(S)}(\Gamma(-t); f_0)$.

In this way, we can calculate the numerical value of $I$ for each trajectory and check whether or not $\langle \exp(-I) \rangle_{mc}$ is unity. However, there is a slight complication here; trajectories with large negative $I$ are rare, but they contribute greatly to $\langle \exp(-I) \rangle_{mc}$. Thus, in order to avoid large numerical error in the computation of $\langle \exp(-I) \rangle_{mc}$ that may
result from the inclusion of too many such rare trajectories, we divided the range of values of \( I \) into discrete intervals, and removed from consideration all trajectories whose values of \( I \) fell inside such intervals that contained fewer than a certain minimum number of data points. In this way, we obtained the normalized distribution function \( \Pi(I) \), which is plotted in Fig. 1. Using the data contained herein, for example, we obtain \( \langle \exp(-I) \rangle_{mc} = 1.03 \).

However, the value obtained for \( \langle \exp(-I) \rangle_{mc} \) in this manner depends on how we divide the range of values of \( I \) into intervals. (In fact, without changing the shape of \( \Pi(I) \) shown in Fig. 1 significantly, we can make \( \langle \exp(-I) \rangle_{mc} \) identically equal to 1.) It is thus necessary to find a better method to determine the value of \( \langle \exp(-I) \rangle_{mc} \) from our data. One such method is to consider the asymmetry around the peak value of the function \( \Pi(I) \). As seen in Fig. 1, it is expected that the equality

\[
\log \Pi(I) - \log \Pi(-I) = I
\]

holds. That is, \( \Pi(I) \) should possess the symmetry described by the fluctuation theorem \( \mathcal{F} \). Then, since \( \Pi(I) \) can be derived from \( \mathcal{F} \), and since the situation depicted in fig. 2 seems to be independent of the manner in which we treat the data, we conclude that \( \Pi(I) \) holds.

Finally, we present a theoretical argument for \( \Pi(I) \). We note, however, that this argument lacks mathematical rigor.

Let us consider \( M \) trajectories whose initial conditions at \( t = \tau_- \) are sampled from the microcanonical ensemble, where \( M \) is a sufficiently large number. Here, in order to simplify the theoretical arguments, we consider the microcanonical ensemble to be defined by the uniform measure on the region between two energy surfaces with energies \( E_0 \) and \( E_0 + \delta E \), where \( \delta E \ll E_0 \).

We divide the phase space into small cells \( \{ \Delta_i \}_{i=1}^\Omega \), each of which has volume \( \epsilon \). We also discretize time as \( t_n = n(\tau_+ - \tau_-) / N + \tau_- \), where \( 0 \leq n \leq N \). We can characterize a trajectory by a set of integers \( (i_0, \ldots, i_N) \), where the phase space point on the trajectory at time \( t_n \) is included in the cell \( \Delta_{i_n} \). We then define the path probability \( P(i_0, \ldots, i_N) \) as the ratio of trajectories characterized by \( (i_0, \ldots, i_N) \) on the set of \( M \). The probability \( p(i_n, t_n) \) of finding the phase space point of an arbitrary one of the \( M \) trajectories in the cell \( \Delta_{i_n} \) at time \( t_n \), is given as the sum of \( P(i_1, \ldots, i_N) \) over all configurations \( (i_1, \ldots, i_{n-1}, i_n, i_{n+1}, \ldots, i_N) \). We note that \( p(i_n, t_n) \) can be interpreted as the time evolution of the distribution function for \( M \) phase space points which are sampled from the microcanonical ensemble at \( t = \tau_- \).

When \( \tau_+ - \tau_- \) is sufficiently large, phase space points on the \( M \) trajectories at time \( t_N \) may spread over the semi-unstable space in the \( i_N \)th cell, subject to the relation \( p(i_N, t_N) \neq 1 \). Therefore, it is expected that \( P(i_0, \ldots, i_N) \) can be expressed as

\[
P(i_0, \ldots, i_N) = \Lambda^{(B)}(i_0, \ldots, i_N)p(i_N, t_N),
\]

where \( \Lambda^{(B)}(i_0, \ldots, i_N) \) is the probability of finding an arbitrary one of the trajectories that are in the semi-unstable space in the \( i_N \)th cell at time \( t = t_N \) to be characterized by \( (i_0, \ldots, i_N) \). Then we introduce the similarly defined quantity \( \Lambda^{(F)}(i_0, \ldots, i_N) \) as the probability of finding an arbitrary one of the trajectories that are in the semi-unstable space in the \( i_0 \)th cell at time \( t = t_0 \) to be characterized by \( (i_0, \ldots, i_N) \). Then, using (20), we have the trivial identity

\[
\sum_{(i_0, \ldots, i_N)} P(i_0, \ldots, i_N) \frac{\Lambda^{(F)}(i_0, \ldots, i_N)p(i_0, t_0)}{\Lambda^{(B)}(i_0, \ldots, i_N)p(i_N, t_N)} = 1.
\]

Now, we conjecture that there is an appropriate limit in which \( \Lambda^{(F)}(i_0, \ldots, i_N) \) and \( \Lambda^{(B)}(i_0, \ldots, i_N) \) approach \( \exp(-\int_{\tau_-}^{\tau_+} \sum_{i=1}^2 \lambda_i^{(F)}(t)) \) and \( \exp(-\int_{\tau_-}^{\tau_+} \sum_{i=1}^2 \lambda_i^{(B)}(t)) \), respectively. Also, from Liouville’s theorem, we know that \( p(i_0, t_0) = p(i_N, t_N) \) holds in the limit \( \epsilon \to 0 \). Therefore, it is reasonable to expect that \( \Pi(I) \) can be derived from (21).

In summary, we have presented numerical evidence for the validity of the non-equilibrium equality \( \Pi(I) \) together with a theoretical argument.

In a previous paper, by numerically studying a Fermi-Pasta-Ulam model with a time-dependent nonlinear term \( \mathcal{F} \), we have found that the Boltzmann entropy difference has a certain relation to the excess information loss \( H_{ex} \). In the billiard model we study presently, \( H_{ex} \) is given by the time integration of \( \Lambda^{(F)}(t) - \Lambda^{(B)}(\Gamma(t); f_1) \) over the region \( t > t_0 \). Therefore, \( I \) is expected to be related to the Boltzmann entropy difference in the thermodynamic limit. Indeed, it has been conjectured that these quantities are equal in the thermodynamic limit \( \mathcal{F} \). Direct numerical evidence supporting this conjecture will be presented elsewhere, together with a complete theory.

Our study is apparently related to the fluctuation theorem, as indicated by the fact that our data apparently satisfy \( \mathcal{F} \). However, it should be pointed out that the entropy production ratio in thermostat models is given by the phase space volume contraction ratio, which is related to \( \lambda_i^{(F)} - \lambda_i^{(B)} \), not \( \Lambda^{(B)} \). Therefore, in extending our...
analysis to non-equilibrium steady states, the irreversible information loss defined by (17) does not become the entropy production. Rather, we believe that this comes to represent a certain quantity related to steady state thermodynamics, which was proposed phenomenologically by Oono and Paniconi [10].

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[1] E. H. Lieb and J. Yngvason, Phys.Rep. 310, 1, (1999).
[2] C. Jarzynski, Phys. Rev. E 56, 5018, (1997); Phys. Rev. Lett. 78 2690 (1997).
[3] G. E. Crooks, Phys. Rev. E 60 , 2721, (1999).
[4] D. J. Evans, E. G. D. Cohen and G. P. Morriss, Phys. Rev. Lett., 71, 2401, (1993).
[5] G. Gallavotti and E. G. D. Cohen, J. Stat. Phys., 80, 931, (1995); Phys. Rev. Lett., 74 2694, (1995).
[6] J. Kurchan, J. Phys. A 31, 3719, (1998); J. L. Lebowitz and H. Spohn, J. Stat. Phys. 95, 333, (1999).
[7] C. Maes, J. Stat. Phys. 95, 367, (1999).
[8] S. Sasa and T. S. Komatsu, Phys. Rev. Lett., 82, 912, (1999).
[9] S. Sasa and T. S. Komatsu, Prog. Theor. Phys., 103, 1, (2000).
[10] Y. Oono and M. Paniconi, Prog. Theor. Phys. Suppl., 130, 29 (1998).
FIG. 1. The normalized distribution function $\Pi(I)$. The values of $E_0$, $f_0$, $f_1$, $\eta$ and $\tau \pm t_0$ are here 1.0, 0, 0.5, 0.02 and $\pm 400$, respectively. We construct a histogram by dividing the interval $[-5, 5]$ into 50 boxes for the 9964 samples considered and removing boxes in which the number of data points is less than 25.
FIG. 2. \( \log \Pi(I) - \log \Pi(-I) \). The dotted line corresponds to \( \log \Pi(I) - \log \Pi(-I) = I \).