Dynamical Instability and Transport Coefficient in Deterministic Diffusion

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We construct both normal and anomalous deterministic biased diffusions to obtain the Einstein relation for their time-averaged transport coefficients. We find that the difference of the generalized Lyapunov exponent between biased and unbiased deterministic diffusions is related to the ensemble-averaged velocity. By Hopf’s ergodic theorem, the ratios between the time-averaged velocity and the Lyapunov exponent for single trajectories converge to a universal constant, which is proportional to the strength of the bias. We confirm this theory using numerical simulations.

Introduction.—Intrinsic randomness of time-averaged observables is of great interest in non-equilibrium statistical mechanics. Equilibrium systems are characterized by a few macroscopic observables, which are the time averages of microscopic observation functions. Macroscopic observables fluctuate around their ensemble averages in an equilibrium state. This means that the time averages of microscopic observation functions converge to their ensemble averages. In contrast, macroscopic observables such as the diffusion coefficient and fluorescence intensity cannot converge to a constant but show large fluctuations in non-equilibrium (non-steady) phenomena such as anomalous diffusions and intermittent phenomena \([1, 2]\). In particular, diffusion coefficients of biological molecules in cells \([1, 2]\) and the fluorescence times in single nanocrystals \([3]\) show large fluctuations, indicating ergodicity breaking.

Such intrinsic randomness of time-averaged observables is known to be universal in models characterized by power-law trapping-time distributions with divergence means \([4, 5]\). A typical example is a continuous time random walk (CTRW), which is a random walk with a random continuous trapping-time. In fact, CTRWs with infinite mean trapping-times show intrinsic randomness of the diffusion coefficient \([3, 4]\). Although ergodicity, i.e., time average being equal to the ensemble average, does not hold in such systems, time averages converge in distribution. This phenomenon is called distributional ergodicity \([10, D]\).

In dynamical systems, distributional ergodicity is known to be the ergodicity in infinite measure systems because dynamical systems relating to stochastic models with infinite mean trapping-times have infinite invariant measures \([11]\). In infinite measure systems, the time average for an observation function converges in distribution. The distribution of the time average is determined by properties of the observation function \([6]\). In particular, the distribution of the time average of an \(L^1(\mu)\) function \(f(x)\) converges to the Mittag-Leffler distribution \([12]\):

\[
\frac{1}{a_n} \sum_{k=0}^{n-1} f \circ T^k \Rightarrow M_\alpha,
\]

provided that \(\int f d\mu \neq 0\), where \(M_\alpha\) is a random variable with a Mittag-Leffler distribution of order \(\alpha\), and \(\Rightarrow\) denotes the convergence in distribution. The sequence \(a_n\) is called the return sequence, which is relevant to non-stationarity. In deterministic subdiffusion, where the mean square displacement grows sublinearly \((x_n^2) \propto n^\alpha\), the scaling of \(a_n\) is the same as \(a_n^{-\alpha}\).

In diffusion processes, an external force \(F\) generates a drift \(V\). In general biased random walks including anomalous diffusion, the Einstein relation,

\[
V = \frac{FD}{2k_B T},
\]

holds \([13]\), where \(D\) is the diffusion coefficient under no bias, \(k_B\) is the Boltzmann constant, and \(T\) is the temperature. Diffusion properties in hyperbolic chaotic dynamical systems are well known. Using the escape rate formula, one can show that the diffusion coefficient is equal to the difference between the Lyapunov exponent and Kolmogorov-Sinai entropy \([14]\). Moreover, in a Lorentz gas, the largest Lyapunov exponent is suppressed by an external field and there is a relation between the Lyapunov exponents and a bias \([13, 15]\). However, little is known about the relation between dynamical instability and the transport property under a bias.

In this Letter, we derive a dynamical system for arbitrary biased and unbiased CTRWs. Furthermore, we explain the linear response to a small bias and the Einstein relation in general deterministic diffusions. Using the Lyapunov exponent, we obtain a relation between the macroscopic transport coefficient and the microscopic chaos in a deterministic subdiffusion. In particular, we relate the ensemble-averaged velocity to the difference of dynamical instabilities between an unbiased and a biased dynamical system. Using Hopf’s ratio ergodic theorem, we show that the ratio between the time-averaged velocity and the Lyapunov exponent converges to a universal constant. Moreover, we find that the universal constant is proportional to a bias, and the proportional constant is determined by the diffusion coefficient and the Lyapunov exponent under no bias.

Deterministic biased diffusion model.—Dynamical systems exhibiting diffusion are represented by one-dimensional map \(T(x)\) with translational symmetry,
The time-averaged drift coefficient is defined by \( \overline{\langle \delta x_m(N) \rangle}_F = (p - q) \langle N \rangle_F/m \). In finite measure cases, the time-averaged diffusion coefficient is equal to the ensemble-averaged one. The ensemble-averaged drift \( \langle \delta x_m \rangle_F \) is given by \( \langle \delta x_m \rangle_F = \langle x_m - x_0 \rangle_F \), where \( \langle \cdot \rangle_F \) refers to the ensemble average under a bias \( c \neq 0.375 \).

Let \( N_m \) be the total number of jumps until time \( m \), then we have \( \langle \delta x_m \rangle_F = (p - q) \langle N \rangle_F \). Here we assume that the injection to the set \([-1/2, -1/4] \cup (1/4, 1/2] \) is uniform (Assumption A). This assumption is exact when the map is a piecewise linear map. It follows that \( p = 2 - 4c \) and \( q = 4c - 1 \). In normal diffusion, \( \langle N \rangle_F \) is given by \( \mu(J^c) \), where \( \mu \) is an invariant measure of \( R(x) \) and \( J = [-1/4, 1/4] \). In subdiffusion, \( \langle N \rangle_F \propto m^\alpha \). Then, we have

\[
\langle \delta x_m(N) \rangle_F = (p - q) \sum_{k=0}^{N-1} \frac{\langle N_{k+m} \rangle - \langle N_k \rangle}{N} \approx \langle \bar{V} \rangle_F/m,
\]

where we define the time-averaged velocity by \( \bar{V} \equiv \delta x_m(N)/m \).

Let \( p = W_0 e^{-F/(2k_BT)} \), \( q = W_0 e^{F/(2k_BT)} \), and \( \Delta n(k) \) be the total number of jumps in the interval \([k, k + m] \), so that \( \langle x_{k+m} - x_k \rangle_F \approx (p - q) \langle \Delta n \rangle_F \). Here we assume \( \langle \Delta n \rangle_F = K \langle \Delta n \rangle \) (Assumption B). \( K \) does not depend on \( c \) for a small bias because the scaling of \( \langle \Delta n \rangle_F \) is the same for all \( c \). It follows that \( \langle x_{k+m} - x_k \rangle_F = K(p - q) \langle \Delta n \rangle \approx K(p - q) \langle (x_{k+m} - x_k)^2 \rangle \). We have

\[
\langle \bar{V} \rangle_F = K \langle \bar{D} \rangle \varepsilon,
\]

where \( \varepsilon = 3 - 8c \). Thus, we obtain the Einstein relation,

\[
\langle \bar{V} \rangle_F = \frac{\langle \bar{D} \rangle F'}{2k_BT}, \quad F \to 0,
\]

where \( F' = KF \), which is not equal to \( F \). It seems that the Einstein relation is violated. However, the change in the waiting time distribution due to the bias results in the violation of the Einstein relation. Therefore, the Einstein relation holds under the bias \( F' \), because the difference between the waiting time distributions for the right and the left does not generate a drift. We note that the ensemble average in the Einstein relation is essential in anomalous subdiffusion because the time-averaged transport coefficients \( \bar{D} \) and \( \bar{V} \) are intrinsically random. When the time-averaged velocity \( \bar{V} \) and the time-averaged diffusion coefficient \( \bar{D} \) are measured independently, \( \bar{V}/\bar{D} \) becomes random, namely, the effective temperature, \( \bar{D}/2k_BT \), becomes random [20].

Relationship between the Lyapunov exponent and the velocity for single trajectories.—The Lyapunov exponent is defined by

\[
\overline{\lambda}(N, x_0) = \frac{1}{N} \left[ \sum_{k=0}^{N-1} \ln |T'(x_k)| \right].
\]
By Hopf’s ergodic theorem \[12\],

\[
\frac{\sum_{k=0}^{n-1} f_m(T^k x)}{\sum_{k=0}^{n-1} g(T^k x)} \to C_m = \int_0^{1/2} f_m d\mu / \int_0^{1/2} g d\mu
\]

(9)

holds for almost all initial points of \(x\), where \(f_m(x) = T^m(x) - x\) and \(g(x) = \ln |T'(x)|\). Therefore, the time-averaged velocity \(\overline{\nabla} (N; x) \equiv \overline{\delta x_m} / m\) and the Lyapunov exponent \(\overline{\lambda} (N; x)\) satisfy the following relation, \(\overline{\nabla} (N; x) / \overline{\lambda} (N; x) \to C_m / m\) as \(N \to \infty\) for almost all \(x\). Since \(\overline{\delta x_m} (N) \propto m\) for a large \(m\), \(C_m / m\) does not depend on \(m\). Let \(C_m / m\) equal \(\chi_V\), then we can obtain the relation between the velocity and the Lyapunov exponent for almost all initial points of \(x\):

\[
\overline{\nabla} (N; x) / \overline{\lambda} (N; x) \to \chi_V \quad \text{as} \quad N \to \infty.
\]

(10)

In general, the ensemble average of the Lyapunov exponent decreases with increase in the ensemble-averaged velocity (see Fig. 3). Nevertheless, the time-averaged velocity is proportional to the Lyapunov exponent. The constant \(\chi_V\) is a universal constant, which does not depend on an initial point. Using the ensemble average and Eq. (6), we obtain

\[
\chi_V = \frac{\overline{\nabla} (\bar{\lambda})}{\overline{\lambda} (\bar{\lambda})} = \frac{K(\bar{\lambda})}{\overline{\lambda}} = \varepsilon.
\]

(11)

**Difference of the Lyapunov exponent.**—We consider the difference of the generalized Lyapunov exponent between an unbiased and a biased dynamical system. The generalized Lyapunov exponent is the ensemble average of the normalized Lyapunov exponent \[11, 21\]

\[
\lambda \equiv \left\langle \lim_{n \to \infty} \frac{1}{a_n} \sum_{k=0}^{n-1} g(x_k) \right\rangle,
\]

(12)

where \(\langle \rangle\) represents the ensemble average of the initial points. Note that the density is absolutely continuous with respect to the Lebesgue measure and satisfies the condition \(\langle g(x_0) \rangle < \infty\). The assumption B, \(\langle \Delta n (k) \rangle_F = K(\Delta n (k))\), means that the statistical property of the reinsertion to the indifferent fixed points is almost the same. That is, the generalized Lyapunov exponent restricted to \(J = [-1, 1] / 2\) is almost the same. The difference of the generalized Lyapunov exponent, \(\Delta \lambda\), is defined by \(\Delta \lambda = \langle \overline{\lambda} (x) \rangle / \langle \overline{\lambda} \rangle \).

By assumption A and B,

\[
\Delta \lambda = \frac{1}{a_n} \sum_{k=0}^{n-1} (\langle g(x_k) 1_{J_c} (x_k) \rangle - \left\langle g_c (x_k) 1_{J_c} (x_k) \right\rangle_F).
\]

(13)

Thus,

\[
\Delta \lambda = \int_{J_c} g(x) d\mu - \int_{J_c} g_c (x) d\mu = \Delta \lambda_{J_c} J_c^c (J_c).
\]

(14)

where \(\Delta \lambda_{J_c}\) is the difference of the generalized Lyapunov exponent restricted to \(J_c\). Since the injection to \(J_c\) is uniform (Assumption A), we have \(\Delta \lambda_{J_c} = \ln 2 + p \ln p + (1 - p) \ln (1 - p)\). The generalized velocity and its maximum are defined as \(V \equiv \lim_{n \to \infty} \langle \delta x_n \rangle_F / n^\alpha\) and \(V_{\text{max}} = \lim_{n \to \infty} \langle n \delta x_n \rangle_F / n^\alpha\), respectively. We use \(V / V_{\text{max}} = p - q\). Then, the probability \(p\) is written by \(V\) and \(V_{\text{max}}\): \(p = (1 + V / V_{\text{max}}) / 2\). Using \(V\) and \(V_{\text{max}}\), we obtain the relation between the difference of the generalized Lyapunov exponent and the generalized velocity:

\[
\Delta \lambda = \frac{\mu (J_c)}{2} S \left( \frac{V}{V_{\text{max}}} \right),
\]

(15)

where \(S (x) = (1 + x) \ln (1 + x) + (1 - x) \ln (1 - x)\). Therefore, the constant \(\chi_V\) is given by

\[
\chi_V = \frac{K(\bar{\lambda})}{\langle \bar{\lambda} \rangle} \varepsilon + O(\varepsilon^2).
\]

(16)

Note that the proportional constant is determined by the diffusion coefficient and the Lyapunov exponent under no bias.

**Example for deterministic subdiffusion.**—We demonstrate numerical results for deterministic subdiffusion. A piecewise linear map is a good approximation for an intermittent map. We consider the following intermittent reduced map:

\[
R(x) = \begin{cases} 
\frac{z-3/4+c}{z-3/4+c} & x \in \left[ -\frac{1}{4}, -\frac{1}{4} + c \right), \\
\frac{z-3/4+c}{z-3/4+c} & x \in \left[ -\frac{1}{4} + c, -\frac{1}{4} \right), \\
x - 4^{-1} (1-x)^z & x \in \left[ -\frac{1}{4}, 0 \right), \\
x + 4^{-1} z x^z & x \in \left[ 0, \frac{1}{4} \right), \\
x - c & x \in \left[ \frac{1}{4}, c \right), \\
\frac{z-c}{z-c} & x \in \left[ c, 1/2 \right]. 
\end{cases}
\]

(17)

The invariant density of the reduced map is given by \(d\mu = h(x)|x|^{-1} \sigma dx\), which means an infinite invariant measure for \(z \geq 2\). \[22\] Since the observation function of a drift, \(f_m (x)\), is an \(L^1(\mu)\) function and \(\int_0^{1/2} f_m (x) d\mu \neq 0\) \((c \neq 0.375)\), the distributional limit theorem, Eq. 14, holds. In particular, the distribution of the normalized time average of \(f_m (x)\) converges to a Mittag-Leffler distribution:

\[
\frac{1}{a_n} \sum_{k=0}^{n-1} f_m \circ T^k \Rightarrow M_\alpha,
\]

(18)

where the return sequence is given by

\[
a_n \propto \begin{cases} 
n (z = 2) \\
n^\alpha (z > 2). 
\end{cases}
\]

(19)

Moreover, the observation function of the Lyapunov exponent, \(g(x) \equiv \ln |T'(x)| = \ln |R'(x)|\), is also the \(L^1_\alpha (\mu)\)
except for a large exponent and the ensemble-averaged velocity is also valid agreement with theory (Fig. 2). Moreover, the relation of the generalized Lyapunov exponent between unbiased map and the Einstein relation for the time-averaged velocity and the constant $\chi$ are obtained by numerical simulations. $K$ is a fitting parameter ($K \approx 1.12$).

![Graph](image)

**FIG. 2.** (Color online) Einstein relation and constant $\chi_V$ ($z = 2.5$). Circles show the results of numerical simulations. Green lines show the theoretical results obtained by Eq. (6) and (16). Constants $\langle \bar{D} \rangle$ and $\langle \bar{X} \rangle$ are obtained by numerical simulations. $K$ is a fitting parameter ($K \approx 1.12$).

**FIG. 3.** (Color online) Relation between the difference of the generalized Lyapunov exponent and the ensemble-averaged velocity ($z = 2.5$). Circles are the results of numerical simulations. The line is the theoretical curve [15], where $V_{\text{max}}$ and $\mu(J^c)$ are obtained by numerical simulations. In particular, we calculate $\mu(J^c)$ by $\lim_{n \to \infty} \langle \sum_{k=0}^{n} 1_{v}(R^k x)/n \rangle$, and we set $a_n = n^\alpha$.

Thus, the normalized Lyapunov exponent is intrinsically random and its distribution converges to a Mittag-Leffler distribution.

Using numerical simulations, we confirmed the Einstein relation and the constant $\chi_V$, which are in good agreement with theory (Fig. 2). Moreover, the relation between the difference of the generalized Lyapunov exponent and the ensemble-averaged velocity is also valid except for a large $V$ (Fig. 3). The generalized Lyapunov exponent is maximized at $V = 0$ and decreased according to the increase in $|V|$.

**Conclusion.**—We derive dynamical systems corresponding to CTRWs. In a biased model, we obtain the Einstein relation for the time-averaged velocity and the time-averaged diffusion coefficient. Moreover, the difference of the generalized Lyapunov exponent between unbiased and biased dynamical systems is represented by the ensemble-averaged velocity. Using Hopf’s ergodic theorem, we find that the ratio between the time-averaged velocity and the Lyapunov exponent converges to a universal constant. The universal constant is proportional to bias and the proportional constant is given by the diffusion coefficient and the Lyapunov exponent without a bias. In general, the ensemble-averaged velocity is represented by the probability $p$: $V = (2p - 1)V_{\text{max}}$, and $p = \mu(J^c)/\mu(J^c)$, where $J^c = [c, 1/2]$. The relation between $\Delta \lambda$ and $V$ will be universal if the map on cell, $[-1/2 + L, L + 1/2]$, is continuous because $\Delta \lambda$ is related to $\mu(J^c)/\mu(J^c)$. Moreover, when the derivative of the map on the interval representing bias is the same as that of the unbiased map, the constant $K$ is almost unity.

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the mean of the total number of jumps $\langle \Delta n(k) \rangle$.. 

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