Extended Einstein relations with a complex effective temperature in a one-dimensional driven lattice gas

Kumiko Hayashi and Shin-ichi Sasa

Department of Pure and Applied Sciences, University of Tokyo, Komaba, Tokyo 153-8902, Japan
(Received 20 April 2004; revised manuscript received 4 February 2005; published 28 April 2005)

We carry out numerical experiments on a one-dimensional driven lattice gas to elucidate the statistical properties of steady states far from equilibrium. By measuring the bulk density diffusion constant D, the conductivity σ, and the intensity of density fluctuations, χ, we confirm that the Einstein relation $D\chi = \sigma T$, which is valid in the linear response regime about equilibrium, does not hold in such steady states. Here, T is the environment temperature and the Boltzmann constant is set to unity. Recalling that the Einstein relation provided the first step in the construction of linear response theory, we attempt to extend it to a generalized form valid in steady states far from equilibrium. In order to obtain new relations among measurable quantities, we define a complex effective temperature $\Theta - i\Phi$ from studying the static response of the system to a slowly varying potential in space. Replacing T in the Einstein relation by the real part of the effective temperature Θ, we numerically confirm that the relation $D\chi = \sigma\Theta$ holds in the nonequilibrium steady states far from equilibrium that we study. In addition to this extended form, we find the relation $(L/2\pi)c\chi = \sigma\Phi$, where c represents the propagation velocity of density fluctuations.

I. INTRODUCTION

In 1905, Einstein derived the relation $D = \mu T$ between the diffusion constant D for noninteracting Brownian particles suspended in an equilibrium fluid of temperature T and mobility μ with respect to an external force [1]. (Here, the Boltzmann constant is set to unity.) This relation is now called the "Einstein relation." Through the development of linear response theory, the original Einstein relation was extended to the form

$$D\chi = \sigma T, \qquad (1)$$

which is valid for interacting many-body systems [2]. Here, D should be considered as the bulk density diffusion constant, χ is the intensity of density fluctuations, and σ is the conductivity.

The Einstein relation is a universal relation in the linear response regime about equilibrium. It represents the first step in the construction of nonequilibrium statistical mechanics in the linear response regime. With this in mind, if the Einstein relation can be extended to some form valid for nonequilibrium steady states (NESS's) far from equilibrium, realizing an understanding of this form will be an important step in the construction of a statistical mechanical theory of NESS's.

With this motivation, because it is simpler to study one-particle NESS systems than many-body systems, we previously analyzed a one-particle Langevin equation with a tilted periodic potential [3]. In that study, it was found that there exists an extended Einstein relation with an effective temperature that can be measured independently of the diffusion constant and the differential mobility. Then, it is natural to ask whether that result for a Brownian particle in NESS's can be extended to many-body interacting systems. In the present paper, we address this question by studying a one-dimensional driven lattice gas (DLG) [4–6] as an example of a many-body interacting system.

II. MODEL

Let η_x be an occupation variable defined on each site x of a one-dimensional periodic lattice $x = 1, 2, \ldots, L$. The variable η_x takes the value 1 if the xth site is occupied by a particle and 0 if it is empty. In order to describe the model simply, we introduce the variable η_{L+1}, which is assumed to be equal to η_1. The array of occupation variables $(\eta_1, \ldots, \eta_L)$ is denoted by η and called the "configuration."

The time evolution of η is described by the following rule: At each time step, randomly choose a nearest-neighbor pair x and $x+1$, where $1 \leq x \leq L$, and exchange the values of η_x and η_{x+1} with probability $c(x; \eta)$ given by $c(x; \eta) = \alpha e^{-\beta Q(\eta \to \eta^x)/2}$, where η^x is the configuration obtained from η through this exchange, $\beta = 1/T$ is the inverse temperature of the environment, and $Q(\eta \to \eta^x)$ represents the heat absorbed from the heat bath as a result of the change of configuration $\eta \to \eta^x$ in one Monte Carlo step (MCS). The constant α is determined so that $c(x; \eta) \leq 1$. The particle number $N = \Sigma_{x=1}^L \eta_x$ is conserved throughout the time evolution, and the averaged density $\bar{\rho} = N/L$ is a parameter of the model.

In this paper, we study the DLG for which

$$Q(\eta \to \eta') = H_0(\eta') - H_0(\eta) - E\sum_{x=1}^{L} j_x(\eta \to \eta'), \quad (2)$$

where E is a constant driving force, $H_0(\eta)$ is the equilibrium Hamiltonian $H_0(\eta) = -\Sigma_{x=1}^L \eta_x \eta_{x+1}$, and $j_x(\eta \to \eta')$ is the net number of particles hopping from x to $x+1$ for the configuration change $\eta \to \eta'$ in one Monte Carlo step. In the argument below, $\langle \, \rangle_E^s$ represents the statistical average in a NESS with driving force E.

Throughout this paper, we fix $\beta = 0.5$, and the numerical parameter α introduced in the exchange probability $c(x; \eta)$ is set to $\exp(-3\beta)$. This value is chosen so that $c(x, \eta) \leq 1$ in the case $E \leq 5$. As a typical example of a NESS far from

equilibrium, we study this model with $E=4$, and we consider the cases $\bar{\rho}=19/64$ and 0.5, with $L=64$, 128, and 256. We remark that because we attempted to evaluate precisely measurable quantities introduced in the next section, it was hard to obtain data in the case $L>256$.

III. EINSTEIN RELATION

Because we have little knowledge regarding relations characterizing NESS's of the DLG, let us start by investigating the validity of the Einstein relation (1) by defining the quantities σ, χ, and D for this model. First, using the averaged current $\bar{J}_E$, which is defined by

$$\bar{J}_E = \frac{1}{L}\left\langle \sum_{x=1}^{L} j_x(\eta \rightarrow \eta') \right\rangle_E^s, \tag{3}$$

the conductivity σ is expressed as

$$\sigma = \frac{d\bar{J}_E}{dE}. \tag{4}$$

Second, the intensity of large scale density fluctuations is defined by

$$\chi(L) = \langle |\hat{\eta}_1|^2 \rangle_E^s, \tag{5}$$

where

$$\hat{\eta}_n(t) = \frac{1}{\sqrt{L}}\sum_{x=1}^{L} \eta_x(Lt)e^{i(2\pi n/L)x}. \tag{6}$$

Third, the density diffusion constant D is defined as the coefficient of the diffusion term of the evolution equation describing the averaged behaviors of the density field. As an example of such behaviors, we consider the time evolution of the density field after a slowly varying weak potential V_x is turned on at $t=0$ in the case that the system is in a steady state. Here V_x is given by

$$V_x = \frac{1}{\sqrt{L}}\hat{V}_1 e^{-i(2\pi/L)x} + \text{c.c.}, \tag{7}$$

where c.c. denotes the complex conjugate and $\hat{V}_1$ is a complex number satisfying $|\hat{V}_1|/\sqrt{L} \ll 1$.

The averaged behavior in this case is represented approximately by the time evolution of a quantity $\langle \hat{\eta}_1(t) \rangle_E^V$, where $\langle \; \rangle_E^V$ denotes the statistical average under the condition that the equilibrium Hamiltonian becomes $H_V(\eta)=H_0(\eta)+\sum_{x=1}^{L}\eta_x V_x$ when $t>0$. We define the response function against V_x as

$$R(t) = -\lim_{|\hat{V}_1| \to 0} \frac{\langle \hat{\eta}_1(t) \rangle_E^V}{\hat{V}_1}. \tag{8}$$

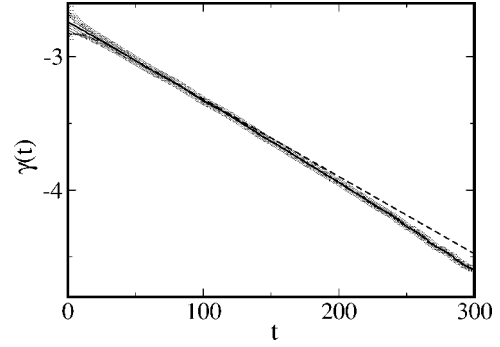In order to see the behavior of $R(t)$, in Fig. 1, we plot

FIG. 1. $\gamma(t)$ is plotted with error bars in the case $\bar{\rho}=0.5$, $L=64$, and $|\hat{V}_1|/\sqrt{L}=0.1$ [see Eq. (10)]. The slope of the fitted line (the dotted line) in the early stage ($t<150$ MCS) corresponds to $D(2\pi/L)^2$. The slope of $\gamma(t)$ in the late stage ($t>150$ MCS) differs from $D(2\pi/L)^2$.

$$\gamma(t) = \log\left| -\frac{\langle \hat{\eta}_1(\infty) \rangle_E^V}{\hat{V}_1} + \frac{\langle \hat{\eta}_1(t) \rangle_E^V}{\hat{V}_1} \right|. \tag{9}$$

Note that we have checked that $\gamma(t)$ takes the same value for the cases $|\hat{V}_1|/\sqrt{L}=0.05$, 0.1, 0.15, and 0.2. It implies that we can estimate the value of the right-hand side of Eq. (8) within a numerical accuracy. It is seen in Fig. 1 that $\gamma(t)$ has a linear slope in the early-time regime. Therefore, using this linear slope, D is estimated from the form

$$|R(\infty) - R(t)| = \text{const} \times e^{-D(2\pi/L)^2 t} \tag{10}$$

in the early-time regime. (We remark that we cannot deny a possibility that the linear slope shown in the early-time regime might be caused by finite-size effects. This is an unresolved problem.)

Using the above definitions of σ, χ, and D, we confirm the validity of Eq. (1) numerically for the equilibrium case $E=0$. With regard to other relations in the linear response theory, we can derive Eq. (1) from the Green-Kubo relation and the fluctuation response relation, which have been proved for DLG models [7]. Contrastingly, in NESS's for our DLG, we find that the two sides of Eq. (1) differ greatly. Specifically, in the case $\bar{\rho}=19/64$, we have confirmed that $\sigma(L)$ and $\chi(L)$ converge to $\sigma_*=0.032$ and $\chi_*=0.26$ in the limit $L \rightarrow \infty$, while D has the anomalous L dependence $D(L) \propto \sqrt{L}$, as shown in Fig. 2. This anomalous behavior is essentially the same as that reported in Ref. [5]. Also, in the case $\bar{\rho}=0.5$, Eq. (1) is not valid because we have confirmed that $\sigma_*=0.037$ and $\chi_*=0.32$ in the limit $L \rightarrow \infty$, while $D(L) \propto \sqrt{L}$ (see Fig. 2).

Now we ask whether it is possible to obtain an extension of the Einstein relation valid for NESS's of interacting many-body systems by defining an appropriate measurable effective temperature. This question arises naturally, because we have found that such an extended Einstein relation does hold for NESS's of one-particle systems. In this relation, the temperature of the environment, T, is replaced by an effective temperature, which can be measured independently of the other quantities appearing in the Einstein relation [3]. By analogy to that case, we seek to define an effective tempera-
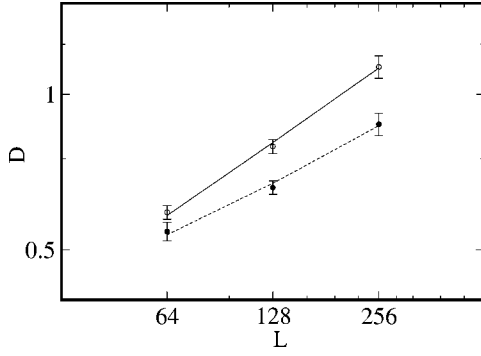
FIG. 2. D as a function of L for the case $\bar{\rho}=19/64$ (solid circles) and $\bar{\rho}=0.5$ (open circles). The dotted line and the solid line represent $0.042\sqrt{L}+0.20$ and $0.068\sqrt{L}+0.0413$, respectively.

ture which when used in place of T in Eq. (1) provides an extended Einstein relation that is valid for NESS's in interacting many-body systems.

IV. EXTENDED EINSTEIN RELATIONS

In a previous study, we showed that the effective temperature appearing in the Einstein relation valid for NESS's of a Brownian particle can be measured by adding a slowly varying potential to the system [3]. In a similar way, we wish to determine an effective temperature by adding to the system a slowly varying potential given by Eq. (7). Due to the influence of this potential, we have $\langle\hat{\eta}_1\rangle_{E,V}^{s}\neq 0$, where $\langle\ \rangle_{E,V}^{s}$ denotes the steady-state average in the system with driving force E and potential V_x. Recalling that the relation

$$\langle\hat{\eta}_1\rangle_{E=0,V}^{s}=-\hat{V}_1\frac{\chi}{T}+o(|\hat{V}_1|) \qquad (11)$$

holds in the equilibrium case, we define the effective temperature $\hat{\theta}_1$ in NESS's as

$$-\lim_{|\hat{V}_1|\to 0}\frac{\langle\hat{\eta}_1\rangle_{E,V}^{s}}{\hat{V}_1}=\frac{\chi(L)}{\hat{\theta}_1}. \qquad (12)$$

Note that in NESS's, the left-hand side of Eq. (12) is a complex number in general. To see this concretely, we show that $\langle\eta_x\rangle_{E,V}^{s}$ under the influence of the potential V_x $=\Delta\sin(2\pi x/L)$ has a component of $\cos(2\pi x/L)$ (see Fig. 3). Expressing explicitly that $\hat{\theta}_1$ is a complex number, we write

$$\hat{\theta}_1=\Theta-i\Phi, \qquad (13)$$

where Θ and Φ are real numbers. In Fig. 5, Θ and Φ are displayed as functions of L in the case $\bar{\rho}=19/64$ and $\bar{\rho}=0.5$. It is seen that we have the anomalous L dependences $\Theta(L)\propto\sqrt{L}$ and $\Phi(L)\propto L$. We remark that $\Phi=0$ in the case $\bar{\rho}=0.5$ (see Fig. 4).

Noting that, from the graphs in Figs. 2 and 5, $D(L)$ and $\Theta(L)$ are both approximately proportional to $\sqrt{L}$, we investigate whether the Einstein relation can be extended to the NESS's by simply replacing T in (1) by $\Theta(L)$. In Fig. 6, we plot $D(L)\chi(L)$ as a function of $\sigma(L)\Theta(L)$ for the cases $\bar{\rho}$
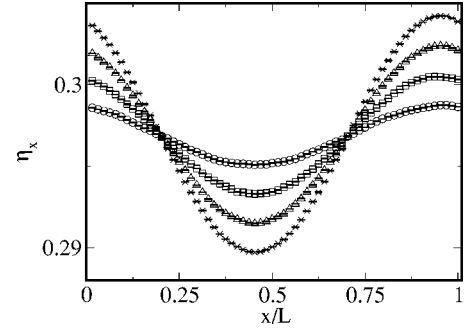

FIG. 3. The profiles of $\langle\eta_x\rangle_{E,V}^{s}$ under the influence of V_x $=\Delta\sin(2\pi x/L)$ in the case $\bar{\rho}=19/64$ and $L=64$. $\Delta=0.1, 0.2, 0.3,$ and 0.4 correspond to the circle, square, triangle, and plus, respectively.

$=19/64$ and 0.5, with $L=64$, 128, and 256. The graph clearly shows that the extended Einstein relation

$$D(L)\chi(L)=\sigma(L)\Theta(L) \qquad (14)$$

holds within the precision of the numerical computations [8].

V. FAILURE OF THE EXTENDED FLUCTUATION RESPONSE RELATION

There are universal relations in the linear response regime about equilibrium, such as the Einstein relation, the
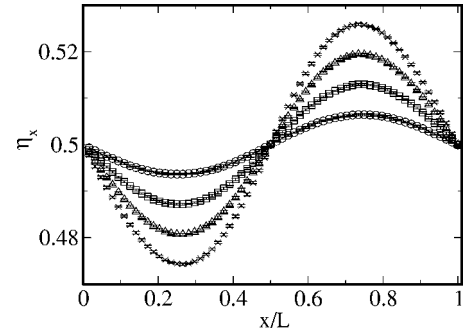

FIG. 4. The profiles of $\langle\eta_x\rangle_{E,V}^{s}$ under the influence of V_x $=\Delta\sin(2\pi x/L)$ in the case $\bar{\rho}=0.5$ and $L=64$. $\Delta=0.1, 0.2, 0.3,$ and 0.4 correspond to the circle, square, triangle, and plus, respectively.
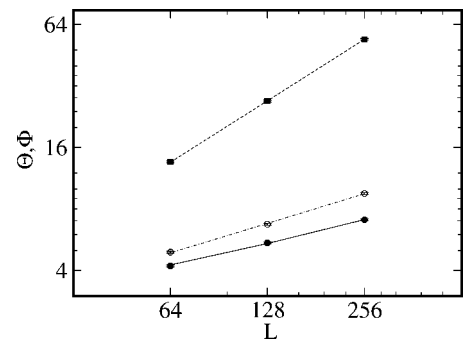

FIG. 5. Θ and Φ as functions of L in the cases $\bar{\rho}=19/64$ (solid symbols) and $\bar{\rho}=0.5$ (open symbols). $\Theta(L)$ and $\Phi(L)$ correspond to the circle and square, respectively. The solid line, the dotted line, and the dash-dotted line represent $0.36\sqrt{L}+1.4$, $0.21L$, and $0.58\sqrt{L}+0.26$. Note that $T=2$.
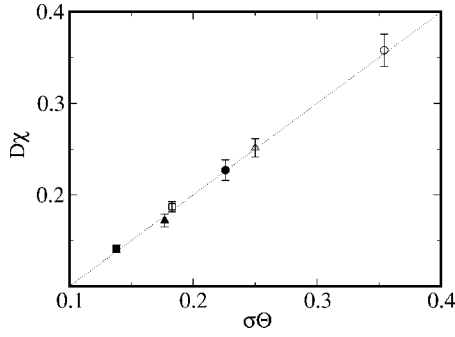
FIG. 6. $D\chi$ as a function of $\sigma\Theta$. The cases $\bar{\rho}=19/64$ and $\bar{\rho}=0.5$ correspond to the solid symbols and the open symbols, respectively. The cases $L=64$, 128, and 256 correspond to the square, triangle, and circle, respectively.

FIG. 7. $R(t)$ as a function of $C(t)$ in the case $\bar{\rho}=0.5$ and $L=64$ during an interval $0 \leqslant t \leqslant 800$ MCS. The slope of the thin line represents Θ^{-1}.

fluctuation-response relation (FRR), and the Green-Kubo relation. One may expect that other relations can be extended in a similar way as was done for the Einstein relation (14) in NESS's far from equilibrium. In this section, we investigate an extension of the FRR.

The FRR connects the time-dependent response function and the time correlation function. In order to define the response function, we consider the situation that the perturbation (7) is applied to the system when $t=0$. The response function $R(t)$ in this situation is defined by Eq. (8). In the equilibrium case, we can prove the FRR

$$R(t) = \frac{1}{T}C(t), \qquad (15)$$

with the time correlation function

$$C(t) = \frac{1}{2}\langle |\hat{\eta}_1(t) - \hat{\eta}_1(0)|^2 \rangle_E^s. \qquad (16)$$

Because the Einstein relation was extended with the replacement of T by $\hat{\theta}_1$, we expect that Eq. (15) can be extended in the form

$$R(t) = \frac{1}{\hat{\theta}_1}C(t). \qquad (17)$$

Specifically, we numerically investigate the validity of Eq. (17) in the case $\bar{\rho}=0.5$ and $L=64$. Because $\Phi=0$ in the case $\bar{\rho}=0.5$, Eq. (17) is rewritten as $R(t)=\Theta^{-1}C(t)$. In Fig. 7, we plot $R(t)$ as a function of $C(t)$ during an interval $0 \leqslant t \leqslant 800$ MCS. It is seen that $R(t)$ deviates from $\Theta^{-1}C(t)$ substantially in an early-time regime ($0 \leqslant t \leqslant 150$ MCS) where the diffusion constant D was defined [see Eq. (10)]. This implies that Eq. (17) is not valid. Note that $R(\infty)=\hat{\theta}_1^{-1}C(\infty)$ holds by the very definition of $\hat{\theta}_1$ given by Eq. (12).

We remark that a generalized version of FRR of the nonlinear Langevin dynamics without the detailed balance condition was presented by several authors [17]. However, in their formalism, a generalized force which defines a response function is chosen so that the simple form of FRR holds, and it seems that their response function cannot be measured directly in experiments. In contrast to the previous studies, we
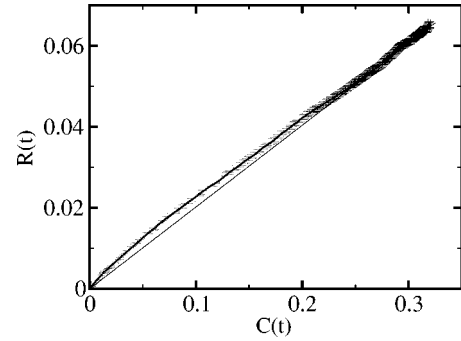
consider a relation between $C(t)$ and $R(t)$ which are measured directly.

VI. INTERPRETATION

In Secs. IV and V, we find that the Einstein relation (14) is extended with the diffusion constant D which is measured from $R(t)$ in the early-time regime and the effective temperature Θ, while the extended FRR (17) is not valid unfortunately. In paragraphs below, we shall provide the phenomenological understanding of validity of Eq. (14) and invalidity of Eq. (17).

The extended Einstein relation (14) can be explained from the following argument. Let $\bar{J}(\rho,E)$ be the averaged particle current in a system with density ρ and driving force E. When the slowly varying potential (7) is applied to this system, first the current should become $\bar{J}(\langle \eta_x \rangle_{E,V}^s, E - dV_x/dx)$, and as a result a diffusive current D, $\langle (\eta_{x+1} - \eta_x) \rangle_{E,V}^s$ should appear so as to make the total current homogeneous in x; that is, it is reasonable to assume that the quantity

$$\bar{J}\left(\langle \eta_x \rangle_{E,V}^s, E - \frac{dV_x}{dx}\right) - D\langle (\eta_{x+1} - \eta_x) \rangle_{E,V}^s \qquad (18)$$

is independent of x in a steady state. This can be rewritten as

$$c\langle \hat{\eta}_1 \rangle_{E,V}^s + i\sigma \frac{2\pi}{L}\hat{V}_1 + i\frac{2\pi}{L}D\langle \hat{\eta}_1 \rangle_{E,V}^s = o\left(\frac{|\hat{V}_1|}{L}, \frac{\langle \hat{\eta}_1 \rangle_{E,V}^s}{L}\right), \qquad (19)$$

where $c=\partial\bar{J}(\bar{\rho},E)/\partial\bar{\rho}$ represents the propagation velocity of density fluctuations. From Eqs. (12) and (19), we obtain

$$\sigma\hat{\theta}_1 = D\chi - i\frac{L}{2\pi}\chi c. \qquad (20)$$

This leads to the extended Einstein relation (14).

Here, we note that a microscopic derivation of Eq. (18) is quite difficult. In particular, we have not been able to show that D defined by Eq. (10) and D in Eq. (18) are identical. In relation to this point, we note that a different value of D is obtained if we consider the time regime $t \geqslant 150$ MCS in Fig. 1. Using this value of D, the relation (14) cannot be con-
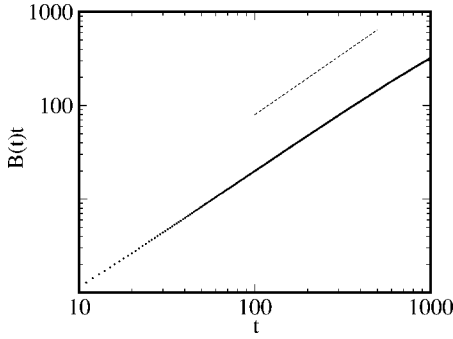
FIG. 8. $B(t)t$ as a function of t in the case $\bar{\rho}=0.5$ and $L=128$. The guided line (the dashed line) represents $B(t)t \propto t^{4/3}$.

FIG. 9. $k^{-1}c\chi$ as a function of $\sigma\Phi$, where $k=2\pi/L$, for the case $\bar{\rho}=19/64$. Note that for the case $\bar{\rho}=0.5$, $c=\Phi=0$. The cases $L=64$, 128, 192, and 256 correspond to the square, triangle, diamond, and circle, respectively. The straight line represents $(L/2\pi)c\chi=\sigma\Phi$. The error bars represent the standard deviations of the statistical samples. In addition to the statistical error bars, there exists a fitting error which is less than 5% of the quantities.

firmed numerically. This result suggests that memory effects in a single-mode description cannot be neglected in the late stage of the relaxation process after the potential is turned on. Because the memory effects arise from a nonlinear coupling between different modes, the simple assumption (18) in NESS's is far from the trivial.

The nontrivial nature of the extended Einstein relation (14) can be seen through the failure of the extended FRR (17). For example, because we cannot observe the exponential decaying regime of $C(\infty)-C(t)$ even in the early-time regime unlike the behavior of $R(\infty)-R(t)$ (see Fig. 1), we cannot define the diffusion constant D properly from the assumption that $\log|C(\infty)-C(t)|=-D(2\pi/L)^2 t+\text{const}$, though in the equilibrium case, the same value of D is obtained whether it is defined from $\log|C(\infty)-C(t)|$ or $\log|R(\infty)-R(t)|$ because of the FRR (15).

The nonexponential decaying behavior of $C(t)$ may be related to a long-time tail of the time correlation function of current fluctuations. Indeed, using the continuity equation, $C(t)$ is expressed by

$$C(t) = \left(\frac{2\pi}{L}\right)^2 \frac{1}{2}\left\langle \left| \sum_{k=1}^{L\tau} \sum_{x=1}^{L} j_x(\eta(k-1) \to \eta(k))e^{i(2\pi/L)x} \right|^2 \right\rangle_E^{\mathrm{s}}. \tag{21}$$

It is expected that the behavior of $C(t)$ in a shorter-time regime than the diffusion time $D^{-1}(2\pi/L)^{-2}$ has common features with that of

$$B(t) = \frac{1}{2}\left\langle \left| \sum_{k=1}^{Lt} \sum_{x=1}^{L} [j_x(\eta(k-1) \to \eta(k)) - \bar{J}_E] \right|^2 \right\rangle_E^{\mathrm{s}}, \tag{22}$$

which is displayed in Fig. 8 in the case $\bar{\rho}=0.5$ and $L=128$. The graph is consistent with the relation $B(t)t \propto t^{4/3}$ which was derived from the theoretical analysis of fluctuating hydrodynamics [5].

We remark that these observations on $R(t)$ and $C(t)$ cannot be explained from the assumption that the time evolution of the density field is described by a linear Langevin equation of $\hat{\eta}_1(t)$, because under this assumption both relations
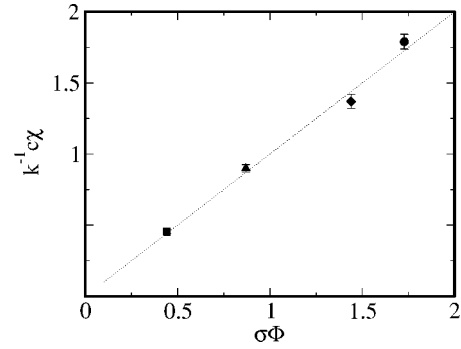
(14) and (17) are derived though Eq. (17) was found not too valid. This implies that the dynamical aspect of the system is too complicated. It may be surprising that the extended Einstein relation holds with the appropriate choice of D.

Finally, from Eq. (20), we find a new relation

$$\frac{L}{2\pi}c(L)\chi(L) = \sigma(L)\Phi(L). \tag{23}$$

We investigated the validity of Eq. (23) in numerical experiments. We numerically measured c from the oscillatory behavior of the time correlation function (16). In one example of this analysis, we considered all t_i satisfying $C(t_i)-C(\infty)=0$, where $t_{i-1}<t_i$. Then, c can be estimated from the relation

$$c\frac{2\pi}{L}(t_{i+1}-t_i) = \pi. \tag{24}$$

We have confirmed that c converges to $c_*=0.17$ in the case $\bar{\rho}=19/64$ in the limit $L\to\infty$. In Fig. 9, we plot $(L/2\pi)c(L)\chi(L)$ as a function of $\sigma(L)\Phi(L)$ for the cases $\bar{\rho}=19/64$, with $L=64$, 128, and 256. (Note that $c=\Phi=0$ for the case $\bar{\rho}=0.5$.) This graph clearly shows that the extended Einstein relation (23) holds within the precision of the numerical computations.

VII. THERMODYNAMIC CONSIDERATION

Here, we devote space to thermodynamic consideration related to our results. We first study the equilibrium case $E=0$ by considering a situation that a perturbation potential is applied to the equilibrium system. When we choose a slowly varying potential, we can regard V_x and $\langle \eta_x \rangle_{E=0,V}^{\mathrm{s}}$ as smooth quantities $V(x)$ and $\rho(x)$. By use of the chemical potential $\mu(\rho,T)$ of the equilibrium system [without the potential $V(x)$], a density profile under the influence of $V(x)$ is determined by a relation that

$$\mu(\rho(x),T) + V(x) = \text{const in } x, \tag{25}$$

which is equivalent to

$$\left(\frac{\partial \mu}{\partial \rho}\right)_T \frac{d\rho}{dx} + \frac{dV}{dx} = 0. \tag{26}$$

Note that the fluctuation relation

$$\left(\frac{\partial \mu}{\partial \rho}\right)_T^{-1} = \frac{\chi}{T} \tag{27}$$

holds in the equilibrium state. As another relation in this situation, we have the total zero-current condition

$$-D\frac{d\rho}{dx} + \bar{J}\left(\rho, -\frac{dV}{dx}\right) = 0. \tag{28}$$

By expanding the second term of Eq. (28) in dV/dx, we obtain

$$D\frac{d\rho}{dx} + \sigma\frac{dV}{dx} = 0. \tag{29}$$

A combination of Eqs. (26), (27), and (29) leads to the Einstein relation (1). In the equilibrium case, we can show just the opposite that a combination of the Einstein relation (1) and the relation (29) derives the fluctuation relation (27) through the relation (25).

In connection with the above-mentioned thermodynamic consideration, we introduce our previous study on a two-dimensional DLG [9]. First, we remark that an appropriate definition of the chemical potential for a NESS is not known unless we use the local equilibrium assumption. Because in NESS's far from equilibrium, the local equilibrium assumption is not valid, we attempted to define a chemical potential without this assumption. Focusing on a density response in a direction perpendicular to the driving force, we defined a nonequilibrium chemical potential by a similar relation with Eq. (25) and constructed an extended thermodynamic function from measurable quantities. As a nontrivial prediction, we showed numerically that the rate function of density fluctuation was determined by this extended thermodynamic function. A theoretical framework behind these observations has been uncovered [10]. We remark that the Einstein relation (1) was also observed in a direction perpendicular to the driving force [11] and that the argument in the previous paragraph can be applied to this case.

In the present paper, we have reported that the extended Einstein relation (14) and the relation (23) hold in NESS's, and a combination of both the relations and Eq. (19) that corresponds to the Fourier transform of Eq. (29) leads to the definition of the effective temperature (12). Because in the case $E=0$ the relation (11) is derived from Eqs. (26) and (27), one might expect that there exists a nonequilibrium chemical potential even for the present NESS's. For example, as a trial, one might propose a nonequilibrium chemical potential $\hat{\mu}_1(\hat{\rho}_1, \hat{\theta}_1)$ as

$$\hat{\mu}_1(\hat{\rho}_1, \hat{\theta}_1) + \hat{V}_1 = 0. \tag{30}$$

However, Eqs. (30) and (12) lead to

$$\left(\frac{\hat{\mu}_1}{\hat{\rho}_1}\right)^{-1} = \frac{\chi}{\hat{\theta}_1}. \tag{31}$$

Because the relation (31) is hard to be interpreted as an extended form of the fluctuation relation (27), the definition (30) seems not to be useful. Taking into consideration that the relation (30) is just one trial, there might be a plausible definition of a chemical potential for NESS's, but we have not found it yet. The difficulty that does not arise in the equilibrium case lies in the wave number dependence of D, as is expected from the system size dependence of D shown in Fig. 2. This wave number dependence is not observed in the equilibrium case and prevents us from pushing ahead further thermodynamic consideration.

VIII. DISCUSSION

Equations (14) and (23) constitute the main results of this paper. In the following, we give five important remarks that are peripherally related to these main results.

First, we give an argument from which to understand a physical meaning of $\hat{\theta}_1$ as the effective temperature. Effective temperatures have been studied mainly in glassy systems [12–16]. The simplest characterization of temperature may be provided by the equipartition. The law of equipartition is regarded as one example of an energy distribution law that can be expressed by the canonical distribution. Out of equilibrium, the equipartition law and the canonical distribution do not hold in general. Indeed, the steady distribution $p_E^s(\eta)$ differs greatly from the canonical one. However, as demonstrated in Refs. [3,13], by constructing measurement methods to extract behavior at some large time and/or length scales, the equipartition law and the canonical distribution are recovered at these scales.

Hypothesizing a similar situation for the NESS's we study, we assume a simple form for the modification of the steady-state measure under the condition that the potential varying slowly in space is added to the system. The form we consider is

$$p_{E,V}^s(\eta) = \frac{1}{Z_V} p_E^s(\eta) e^{-(\hat{\eta}_{-1}\hat{\theta}_1^{-1}\hat{V}_1 + \text{c.c.})} \tag{32}$$

for $|\hat{V}_1| \ll 1$, where Z_V is a normalization constant. From Eq. (32), we can derive Eq. (12), which is the definition of $\hat{\theta}_1$. We believe that the simple form (32), which describes the response of the steady-state measure to this slowly varying potential, is a good starting point to investigate NESS's.

Second, we remark that our main result also holds for the case $H_0(\eta)=0$, which is an example of asymmetric simple exclusion process (ASEP). Specifically, we consider the case $\rho=0.5$ and $L=64$. χ and σ are calculated theoretically as $\chi(L)=0.25$ and $\sigma(L)=0.043$. The diffusion constant $D(L)$ is measured numerically as $D(L)=0.68$ (see Fig. 10). Θ is also measured as $\Theta(L)=3.9$ from Eq. (12). Thus the relation $D(L)\chi(L)=\sigma(L)\Theta(L)$ seems valid. Study of the large-scale behavior of the system might give new insights into the ASEP.
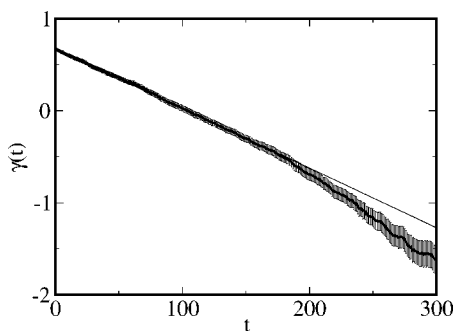
FIG. 10. In the case $H_0(\eta)=0$ (ASEP), $\gamma(t)$ is plotted with error bars in the case $\bar{\rho}=0.5$, $L=64$, and $|\hat{V}_1|/\sqrt{L}=0.1$ [see Eq. (10)]. The slope of the fitted line (thin line) in the early stage ($t < 150$ MCS) corresponds to $D(2\pi/L)^2$.

Third, we remark on a connection with fluctuating hydrodynamics. Note that the system in our numerical experiments may be too small for the dynamical behavior to be described within the framework of fluctuating hydrodynamics, while large enough so that we can check universal relations around equilibrium states. The fact that $D(L) \propto \sqrt{L}$ (see Fig. 2) in such small systems seems to imply that bare parameters appearing in fluctuating hydrodynamics depend on a length scale ℓ at which the hydrodynamic description is defined. [Note that the scaling relation $D(L) \propto \sqrt{L}$ can be derived within the framework of fluctuating hydrodynamics, irrespective of the values of the bare parameters [5].] Thus, it is plausible to conjecture that we need to specify a scale ℓ explicitly so as to have a hydrodynamic description. We do not understand how the formal derivation in Ref. [17] corresponds to this observation.

Fourth, we make a comment on the diffusion of a marked particle. The diffusion is characterized by a tracer diffusion constant, which is not equal to the bulk diffusion constant D defined by Eq. (10). One may question whether the tracer diffusion constant can be involved in a universal relation for NESS's. We have not found such a relation yet, but it may be an interesting future problem to seek it. We note that the tracer diffusion constant does not have the anomalous L dependence in contrast to the case of D.

The final remark we wish to present regards the possibility of an experiment that can check the extended Einstein relations we have proposed. We conjecture that it may be best to study a system in which colloid particles, confined to one dimension, are driven through a periodic array of optical traps [18]. By defining the effective temperature in the same way as done in Eq. (12), the validity of the extended Einstein relations will be checked.

[1] A. Einstein, Ann. Phys. **17**, 549 (1905); *Investigations on the Theory of Brownian Movement* (Dover, New York, 1956).

[2] R. Kubo, Rep. Prog. Phys. **29**, 255 (1966).

[3] K. Hayashi and S. Sasa, Phys. Rev. E **69**, 066119 (2004).

[4] S. Katz, J. L. Lebowitz, and H. Spohn, J. Stat. Phys. **34**, 497 (1984).

[5] H. van Beijeren, R. Kutner, and H. Spohn, Phys. Rev. Lett. **54**, 2026 (1985).

[6] H. Spohn, *Large Scale Dynamics of Interacting Particles* (Springer-Verlag, Berlin, 1991).

[7] K. Hayashi and S. Sasa (unpublished).

[8] There is a puzzle that the extended Einstein relation seems to connect this D with σ, because D is evaluated from the short-time behavior of the system, while σ is measured as the long-time average in the steady state.

[9] K. Hayashi and S. Sasa, Phys. Rev. E **68**, 035104(R) (2003).

[10] S. Sasa and H. Tasaki, e-print cond-mat/0411052.

[11] K. Hayashi (unpublished).

[12] L. F. Cugliandolo, J. Kurchan, and L. Peliti, Phys. Rev. E **55**, 3898 (1997).

[13] L. Berthier and J.-L. Barrat, Phys. Rev. Lett. **89**, 095702 (2002).

[14] A. B. Kolton, R. Exartier, L. F. Cugliandolo, D. Dominguez, and N. Gronbech-Jensen, Phys. Rev. Lett. **89**, 227001 (2002).

[15] I. K. Ono *et al.*, Phys. Rev. Lett. **89**, 095703 (2002).

[16] T. Harada, e-print cond-mat/0310547, Europhys. Lett. (to be published).

[17] G. L. Eyink, J. L. Lebowitz, and H. Spohn, J. Stat. Phys. **83**, 385 (1996), and references therein

[18] P. T. Korda, M. B. Taylor, and D. G. Grier, Phys. Rev. Lett. **89**, 128301 (2002).