Linear response theory in stochastic many-body systems revisited

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Abstract

The Green-Kubo relation, the Einstein relation, and the fluctuation-response relation are representative universal relations among measurable quantities that are valid in the linear response regime. We provide pedagogical proofs of these universal relations for stochastic many-body systems. Through these simple proofs, we characterize the three relations as follows. The Green-Kubo relation is a direct result of the local detailed balance condition, the fluctuation-response relation represents the dynamic extension of both the Green-Kubo relation and the fluctuation relation in equilibrium statistical mechanics, and the Einstein relation can be understood by considering thermodynamics. We also clarify the interrelationships among the universal relations.

Key words: linear response theory, driven lattice gas
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1 Introduction

Let us consider the general class of systems exhibiting the macroscopic flow of some quantity. Familiar examples include electric conduction systems, heat conduction systems and driven colloidal systems. Such systems often exist in states in which the current is stationary. We refer to these states as nonequilibrium steady states. Nonequilibrium steady states are the simplest type of nonequilibrium states. However, even for the class consisting of such simple states, there presently exists no universal framework to calculate macroscopic properties of systems from microscopic information, in contrast to the class of equilibrium states, for which macroscopic properties can be calculated from the partition function of the system, employing the well-established theory of statistical mechanics.
At the present time, there exists a theory of nonequilibrium systems only for the regime very near equilibrium. This so-called linear response theory consists of a set of universal relations, which includes the Green-Kubo relation, the fluctuation-response relation and the Einstein-relation. These relations relate the dynamical properties of fluctuations in systems under equilibrium conditions to linear transport properties of nonequilibrium systems. The validity of these relations has been confirmed by both experimental and theoretical investigations [1].

In recent years, properties regarding fluctuations and linear responses to perturbations have been investigated for nonequilibrium states even outside the linear response regime, in steady state systems [2], aging systems [3,4,5] and other systems [6,7]. Obviously, we cannot expect the relations proved within linear response theory to be generally valid outside the linear response regime. However, there have been several relations proposed and investigated recently that represent extensions of the relations in linear response theory to systems far from equilibrium [8,9,10,11,12,13,14].

We wish to acquire a systematic understanding of these extended relations among fluctuations and response properties, aiming at the construction of a statistical mechanics of nonequilibrium systems far from equilibrium. For this purpose, first it is necessary to grasp the essence of the basic framework of linear response theory, in particular focusing on the elucidation of the interrelations among the linear response relations, thermodynamics and equilibrium statistical mechanics.

Of course, all of the relations in linear response theory can be derived by applying a formal perturbative expansion to quantum or classical mechanical descriptions on the basis of equilibrium statistical mechanics [15,16,17,18,19]. However, such formal derivations of these relations does not illuminate the physical picture (see Section 8). In this paper, instead of applying a formal perturbation theory to quantum or classical mechanical systems, we attempt to elucidate the essence of linear response theory by studying stochastic many-body systems.

Among the various types of stochastic many-body systems, we choose to investigate two kinds of one-dimensional nonequilibrium lattice gases in which particles hop stochastically from one lattice site to another according to a given transition rate [20,21,22,23]. Specifically, we study a driven lattice gas, in which particles are driven by an external driving force in the bulk, and a boundary-driven lattice gas, in which particles are driven by the difference in chemical potential between two particle reservoirs in contact with the boundaries. Although we choose these models for their mathematical simplicity, it is straightforward to apply the method of proof to other stochastic many-body systems, such as Langevin systems that describe the motion of many beads in
This paper is organized as follows. In Section 2, we state our physical point of view and the basic assumptions used in the derivation of the linear response relations. In Section 3, we introduce a one-dimensional driven lattice gas. In Section 4, we present a simple derivation of the Green-Kubo relation, employing a key identity, with which various universal relations characterizing nonequilibrium steady states can be derived. In Section 5, we derive the fluctuation-response relations and elucidate its connection to equilibrium statistical mechanics. In Section 6, we derive the Einstein relation for the model, and clarify the connections among these three universal relations and thermodynamics. In Section 7, we derive the Green-Kubo relation for a boundary-driven lattice gas, which is a different type of nonequilibrium lattice gas, in order to demonstrate the generality of our argument. Finally, in Section 8, we give several important remarks concerning linear response theory.

2 Basic assumption

Let us recall that the macroscopic properties of an equilibrium system can be investigated with statistical mechanics using an effective multi-dimensional variable $\alpha$ and the corresponding effective Hamiltonian $H(\alpha)$. More precisely, in order to obtain such a description, the variable $\alpha$, described statistically, need not constitute a complete set of mechanical variables that specifies the microscopic state in classical or quantum systems. For example, consider a system consisting of many beads suspended in a liquid. In this case, $\alpha$ can be regarded as representing the set of centers of mass of the beads, with $H(\alpha)$ describing the effective interactions between them. The effect of the liquid can be included in this effective Hamiltonian $H(\alpha)$.

Here, we suppose that the set of variables $(\alpha, \Gamma)$ provides a complete mechanical description of the system under consideration. For the bead system, $\Gamma$ is defined so that $(\alpha, \Gamma)$ represents all the positions and conjugate momenta of the atoms composing the beads and the liquid in an adiabatic container.

Now, we consider a nonequilibrium system which is such that the degrees of freedom represented by $\Gamma$ remain in equilibrium, while only those represented by $\alpha$ are in a nonequilibrium state. It is not certain that such an assumption would be valid, and in general the degree of error it introduces would depend on the system we consider. Physically, this assumption seems reasonable in the case that the typical time scale of $\alpha$, $\tau_\alpha$, is much longer than that of $\Gamma$, $\tau_\Gamma$. We consider such a case and introduce a time interval $\Delta t$ satisfying $\tau_\Gamma \ll \Delta t \ll \tau_\alpha$. In the argument below, we refer the subsystem composed of the degrees of freedom $\Gamma$ as the heat bath. Because this heat bath is assumed
to be always in equilibrium, its temperature, $T$, is defined for nonequilibrium states of the remaining degree of freedom.

In order to describe the nonequilibrium states of such systems, we need to determine the time evolution of the variable $\alpha$ on the time scale of the interval $\Delta t$. Due to the separation of time scales represented by the relation $\tau \ll \Delta t$, it is reasonable to assume that $\alpha$ is described by a Markov stochastic process with a transition probability $T(\alpha \to \alpha')$.

The fundamental assumption in this paper is expressed by the local detailed balance condition
\[ \frac{T(\alpha \to \alpha')}{T(\alpha' \to \alpha)} = e^{-\beta Q(\alpha \to \alpha')} \] (1)
where $\beta = 1/T$. Here, the Boltzmann constant is set to unity. The quantity $Q(\alpha \to \alpha')$ represents the energy transferred from this heat bath, which we call heat, during the time evolution symbolized by $\alpha \to \alpha'$ taking place over the time interval $\Delta t$.

In the system under equilibrium conditions, because the energy conservation expressed as $Q(\alpha \to \alpha') = H(\alpha') - H(\alpha)$ should hold, (1) becomes the detailed balance condition of the transition probability:
\[ p^\text{can}(\alpha)T(\alpha \to \alpha') = p^\text{can}(\alpha')T(\alpha' \to \alpha), \] (2)
with respect to the canonical distribution
\[ p^\text{can}(\alpha) = \frac{e^{-\beta H(\alpha)}}{Z}, \] (3)
where $Z$ is a normalization constant. Combining (2) with the normalization condition of the probability, $\sum_{\alpha'} T(\alpha \to \alpha') = 1$, we derive
\[ p^\text{can}(\alpha) = \sum_{\alpha'} p^\text{can}(\alpha')T(\alpha' \to \alpha). \] (4)

This equality implies that (3) is the stationary distribution of $\alpha$. This result is consistent with equilibrium statistical mechanics. Also, it turns out that the detailed balance condition (2) implies time-reversal symmetry in the sense that the two-time joint probability $p^\text{can}(\alpha)T(\alpha \to \alpha')$ is invariant under the exchange of $\alpha$ and $\alpha'$.

By contrast, in the case of a nonequilibrium state, it is not easy to obtain a physical interpretation of (1). We explain the origin of the name local detailed balance condition in Section 3, and demonstrate that all the universal relations can be derived from this assumption in Sections 4, 5, and 6. In the remainder of this section, we explain how the local detailed balance condition (1) places restrictions on the allowed types of interactions with the heat bath.
In order to demonstrate this point explicitly, we consider a many-body bead system in which an external driving force is applied to the beads. We wish to derive the transition probability $T(\{r_j\} \rightarrow \{r'_j\})$ over an infinitesimally small time interval $\Delta t$, using the local detailed balance condition, where $r_i$ ($i = 1, \cdots, N$) represents the position of the $i$-th bead.

First, note that the mechanical force acting on the $i$-th bead is given by

$$F_i(\{r_j\}) = f e_x - \frac{\partial U_0(r_i)}{\partial r_i} - \sum_{j=1; j \neq i}^{N} \frac{\partial U(r_i - r_j)}{\partial r_i}, \quad (5)$$

where $U_0$ is a one-body potential (e.g. a spatially periodic potential), $U$ is the interaction potential between beads, and $f$ is an external driving force.

Then, because the change in momentum is much smaller than the dissipative force in this situation, the averaged motion caused by the force $F_i(\{r_j\})$ is determined by the force balance equation

$$-\gamma(\langle r'_i \rangle - \langle r_i \rangle) + \bar{F}_i \Delta t = 0, \quad (6)$$

where $\gamma$ represents the dissipation constant, and $\bar{F}_i$ is the average of $F_i$ during the transition, given by

$$\bar{F}_i = \frac{1}{2}[F_i(\{r_j(t)\}) + F_i(\{r_j(t + \Delta t)\})]. \quad (7)$$

Under the influence of the interactions with molecules in the liquid, the positions of the beads fluctuate around this averaged motion. Because we choose $\Delta t$ to be much larger than the time scale characterizing the dynamics of the molecules, we expect that these fluctuations exhibit a Gaussian distribution with a dispersion proportional to $\Delta t^{-1}$. That is, it is reasonable to express the fluctuations by the transition probability

$$T(\{r_j\} \rightarrow \{r'_j\}) = \frac{1}{Y} e^{-\Delta t \frac{1}{2b} \sum_{i=1}^{N} |\dot{r}_i - \bar{F}_i|^2}, \quad (8)$$

where $Y$ is a normalization factor, $b$ is a parameter which represents the strength of the interaction with the heat bath, and $\dot{r}_i$ should be interpreted as

$$\dot{r}_i = \frac{r'_i - r_i}{\Delta t}. \quad (9)$$

We wish to determine $b$ in (8) from the local detailed balance condition. In order to do this, we consider the following ratio of transition probabilities:

$$\frac{T(\{r_j\} \rightarrow \{r'_j\})}{T(\{r'_j\} \rightarrow \{r_j\})} = e^{\Delta t \frac{1}{b} \sum_{i=1}^{N} \dot{r}_i \bar{F}_i}. \quad (10)$$

In this expression, it should be noted that the quantity $\Delta t \sum_{i=1}^{N} \dot{r}_i \bar{F}_i$ is the work done by the force $\bar{F}_i$, which is equal to the heat dissipated into the heat
bath [24] during the transition from \( \{ r_i \} \) to \( \{ r'_i \} \). Then, by comparing (10) with the local detailed balance condition (1), we find the relation

\[
b = \gamma T.
\]  

(11)

In this way, we have determined the transition probability (8), with the explicit form of \( b \) from the local detailed balance condition (1).

Note that the stochastic process given by the transition probability (8) can be expressed as

\[
\gamma (r'_i - r_i) = \vec{F}_i \Delta t + \Delta W_i,
\]  

(12)

where \( \Delta W_i \) represents Brownian motion satisfying

\[
\langle \Delta W_i \Delta W_j \rangle = 2b\delta_{ij}\Delta t.
\]  

(13)

Then, taking the limit \( \Delta t \to 0 \), we obtain the Langevin equation

\[
\gamma \dot{r}_i = f e_x - \frac{\partial U_0(r_i)}{\partial r_i} - \sum_{j=1; j \neq i}^{N} \frac{\partial U(r_i - r_j)}{\partial r_i} + \xi_i,
\]  

(14)

where \( \xi_i \) represents zero-mean Gaussian white noise with

\[
\langle \xi_i(t)\xi_j(t') \rangle = 2b\delta_{ij}I\delta(t - t').
\]  

(15)

Here, \( I \) is a unit matrix. The condition (11) is called the fluctuation-dissipation relation of the second kind for the Langevin equation (14) with (15).

3 Model

We can derive all the universal relations in linear response theory for the Langevin equation (14) with (11) and (15). However, this derivation is complicated when mathematical rigor is maintained. Instead of the Langevin model, we study a lattice gas, which also serves as a model of many-body beads systems, to avoid the complicated analysis that is irrelevant to the essence of linear response theory.

In a lattice gas, particles hop stochastically from one lattice site to another at a given transition rate. Particularly, when two or more particles cannot be placed at one site, the equilibrium state is described by a Hamiltonian which is equivalent to that for a spin model with a variable transformation. For mathematical simplicity, the form of the Hamiltonian usually corresponds to the Ising model. In Subsection 3.1, we explain the one-dimensional equilibrium lattice gas. A two or higher dimensional model can be easily interpreted from the one-dimensional case.
A driven lattice gas, introduced in Subsection 3.2, is defined by minimally modifying to the equilibrium lattice gas so that it exhibits nonequilibrium steady states. The model was numerically and theoretically investigated in Refs. [21,22,23].

3.1 One-dimensional equilibrium lattice gas

We first define an occupation variable, $\eta_x$, on each site $x$ in a one-dimensional periodic lattice $x = 1, 2, \cdots, L$. $\eta_x = 1$ when the site $x$ is occupied by a particle and $\eta_x = 0$ if $x$ is unoccupied. A periodic boundary condition is imposed by introducing a boundary site at $x = 0$ and setting $\eta_0 = \eta_L$. The collection of all occupation variables $(\eta_1, \cdots, \eta_L)$ represents the particle positions in the system. We denote $(\eta_1, \cdots, \eta_L)$ as $\eta$, which is referred to as the configuration.

For convenience, we use $\eta^x$ to represent the configuration when the value of $\eta_x$ is replaced with that of $1 - \eta_x$. In a similar way, $\eta^{xy}$ represents the configuration when the values of $\eta_x$ and $\eta_y$ are replaced by $1 - \eta_x$ and $1 - \eta_y$. (Note that the configuration after exchanging the value of $\eta_x$ and $\eta_y$ is represented by this $\eta^{xy}$.) The interaction between the particles is described by the Hamiltonian

$$H_0(\eta) = -\sum_{x=0}^{L-1} \eta_x \eta_{x+1}. \quad \text{(16)}$$

The time evolution of $\eta$ is expressed as follows: At each time step, a nearest neighbor pair $x$ and $y$, $0 \leq x, y \leq L$, is randomly selected and the values of $\eta_x$ and $\eta_y$ are exchanged using the exchange probability $c_0(x, y; \eta)$ that satisfies

$$c_0(x, y; \eta) = c_0(x, y; \eta^{xy}) e^{-\beta Q_0(\eta \rightarrow \eta^{xy})}, \quad \text{(17)}$$

with

$$Q_0(\eta \rightarrow \eta') = H_0(\eta') - H_0(\eta). \quad \text{(18)}$$

$Q_0(\eta \rightarrow \eta^{xy})$ corresponds to the heat absorbed from the heat bath for the configuration change $\eta \rightarrow \eta^{xy}$. We also define $c_0(x, y; \eta) = 0$ for pairs $x$ and $y$ such that $|x - y| \neq 1$. We regard this step as a Monte Carlo step.

Examples of common concrete forms of $c_0(x, y; \eta)$ are the Metropolis method

$$c_0(x, y; \eta) = \min\{1, e^{-\beta Q_0(\eta \rightarrow \eta^{xy})}\} \quad \text{min}\{1, e^{-\beta Q_0(\eta \rightarrow \eta^{xy})}\}, \quad \text{(19)}$$

the heat bath method

$$c_0(x, y; \eta) = \frac{1}{1 + e^{\beta Q_0(\eta \rightarrow \eta^{xy})}}, \quad \text{(20)}$$

and the exponential rule

$$c_0(x, y; \eta) = \text{const.} e^{-\frac{1}{2} \beta Q_0(\eta \rightarrow \eta^{xy})}, \quad \text{(21)}$$
where const. is chosen so as to satisfy the condition that \( c_0(x, y; \eta) \leq 1 \). It can be easily checked that (19), (20) and (21) satisfy (17).

The transition probability \( T_0(\eta \rightarrow \eta') \) for one Monte Carlo step is written as

\[
T_0(\eta \rightarrow \eta') = \frac{1}{L} c_0(x, y; \eta)
\]  

(22)

for \( \eta' = \eta^{xy} \neq \eta \), and \( T_0(\eta \rightarrow \eta) \) is determined by the normalization condition of the probability

\[
\sum_{\eta'} T_0(\eta \rightarrow \eta') = 1.
\]  

(23)

Note that in the argument, \( T_0(\eta \rightarrow \eta') \) is different from \( c_0(x, y; \eta) \); the transition probability, \( T_0(\eta \rightarrow \eta') \), is a function of two configurations, while the exchange probability, \( c_0(x, y; \eta) \), is a function of the sites \( x, y \) and the configuration \( \eta \).

From (17) and (22), we find that \( T_0(\eta \rightarrow \eta') \) satisfies the local detailed balance condition

\[
\frac{T_0(\eta \rightarrow \eta')}{T_0(\eta' \rightarrow \eta)} = e^{-\beta Q_0(\eta \rightarrow \eta')}. 
\]  

(24)

Here, using (18) in this equilibrium case, the condition (24) becomes the detailed balance condition

\[
p^{\text{can}}(\eta) T_0(\eta \rightarrow \eta') = p^{\text{can}}(\eta') T_0(\eta' \rightarrow \eta),
\]  

(25)

with respect to the canonical distribution

\[
p^{\text{can}}(\eta) = \frac{e^{-\beta H_0(\eta)}}{Z} \delta(\sum_{x=1}^{L} \eta_x - N).
\]  

(26)

Here, \( Z \) is a normalization constant, and \( N \) is the total number of particles,

\[
N = \sum_{x=1}^{L} \eta_x,
\]  

(27)

which is conserved through this time evolution. \( \bar{\rho} = N/L \) is introduced to be a parameter of the model. Similar to Section 2, using (25), we can confirm that (26) is the stationary distribution of this model in the equilibrium case.

### 3.2 One-dimensional driven lattice gas

In this subsection, a driven lattice gas that describes a physical situation where the particles are driven by a uniform driving force \( E \) in the bulk is introduced as a simple extended model of the equilibrium lattice gas. First, we define the
net number of particles that hop from $x$ to $x + 1$ in the configuration change $\eta \rightarrow \eta'$ as

$$\Phi_x(\eta \rightarrow \eta') = \eta_x(1 - \eta'_x)\eta'_{x+1}(1 - \eta_{x+1}) - \eta'_x(1 - \eta_x)\eta_{x+1}(1 - \eta'_{x+1}).$$  (28)

Note that $\Phi_x(\eta \rightarrow \eta')$ takes a value in $\{\pm 1, 0\}$. Then, the heat $Q_0$ given in (18) is replaced with

$$Q(\eta \rightarrow \eta') = H_0(\eta') - H_0(\eta) - E \sum_{x=0}^{L-1} \Phi_x(\eta \rightarrow \eta'),$$  (29)

to consider the effect of the driving force on the time evolution rule, because $Q(\eta \rightarrow \eta')$ is interpreted as the heat absorbed from the heat bath for the configuration change $\eta \rightarrow \eta'$ in one Monte Carlo step. Using this replacement, $c_0(x, y; \eta)$ in (17) and $T_0(\eta \rightarrow \eta')$ in (22) are replaced by $c(x, y; \eta)$ and $T(\eta \rightarrow \eta')$, respectively. Then, $T(\eta \rightarrow \eta')$ satisfies the local detailed balance condition

$$\frac{T(\eta \rightarrow \eta')}{T(\eta' \rightarrow \eta)} = e^{-\beta Q(\eta \rightarrow \eta')}.$$  (30)

Here, one may consider whether $Q(\eta \rightarrow \eta')$ given in (29) can be expressed as

$$Q(\eta \rightarrow \eta') = \sum_{x=0}^{L-1} h_x(\eta') - \sum_{x=0}^{L-1} h_x(\eta),$$  (31)

with a local Hamiltonian

$$h_x(\eta) = -\eta_x\eta_{x+1} - Ex\eta_x.$$  (32)

If (31) and (32) were valid, this should correspond to the detailed balance condition, because (30) can be written as

$$T(\eta \rightarrow \eta') e^{-\beta \sum_{x=0}^{L-1} h_x(\eta)} = T(\eta' \rightarrow \eta) e^{-\beta \sum_{x=0}^{L-1} h_x(\eta')}.$$  (33)

However, (31) is valid only when $\eta' = \eta^{x+1}$ with $0 \leq x \leq L - 2$, and is invalid when $x = L - 1$, unless $E = 0$. More generally, when $E \neq 0$, (31) can be satisfied for the configuration changes with one exception, but not for all exchanges, even if we introduce another local Hamiltonian. Due to this property, the condition (30) is called the local detailed balance condition. As shown in the above argument, the local detailed balance condition does not necessarily imply the detailed balance condition, except for the equilibrium case.

Throughout this paper, we regard $L$ Monte Carlo steps as the unit of time, which is the number of Monte Carlo steps necessary for all sites to be selected once on the average. This unit of time is called one MCS (Monte Carlo step per site). Then, we denote the history of the configurations from 0 to $\tau$
MCS as \([\eta] = (\eta(0), \eta(1), \ldots, \eta(L\tau))\). The probability of a history \([\eta]\) in the nonequilibrium steady state, \(P^\text{st}_E([\eta])\), is written as

\[
P^\text{st}_E([\eta]) = p^\text{st}_E(\eta(0))T(\eta(0) \to \eta(1)) \cdots T(\eta(L\tau - 1) \to \eta(L\tau)),
\]

(34)

where \(p^\text{st}_E(\eta)\) is the stationary distribution in the system with the driving force \(E\). Specifically, when \(E = 0\), \(p^\text{st}_E=0\) is identical to \(p^\text{can}(\eta)\) defined in (26). Then, the statistical average of a history dependent quantity \(A\) in the steady state is denoted as

\[
\langle A \rangle^\text{st}_E \equiv \sum_{[\eta]} P^\text{st}_E([\eta])A([\eta]).
\]

(35)

4 Green-Kubo relation

In this section, we provide a simple proof of the Green-Kubo relation for the one-dimensional driven lattice gas. During the derivation, we obtain the key identity given in (44). Using this key identity, we can derive the nonlinear response relation, the fluctuation theorem and the steady state distribution as well as the Green-Kubo relation.

4.1 Main claim

We first define the spatially averaged current per one MCS at time \(t\), \(j(t)\). Because the number of particles moving from the site \(x\) to the site \(x + 1\) from \(t\) to \(t + 1\) is expressed as \(\sum_{k=0}^{L-1} \Phi_x(\eta(Lt + k) \to \eta(Lt + k + 1))\), \(j(t)\) is written as

\[
j(t) \equiv \frac{1}{L} \sum_{x=0}^{L-1} \sum_{k=0}^{L-1} \Phi_x(\eta(Lt + k) \to \eta(Lt + k + 1)).
\]

(36)

Using the steady state current, \(\bar{J} = \langle j \rangle^\text{st}_E\), the conductivity, \(\sigma\), is defined as

\[
\sigma \equiv \lim_{E \to 0} \frac{\bar{J}}{E}.
\]

(37)

Furthermore, for the \(\tau\)-averaged current

\[
J_\tau([\eta]) \equiv \frac{1}{\tau} \sum_{t=0}^{\tau-1} j(t),
\]

(38)

its fluctuation is characterized by

\[
B \equiv \lim_{\tau \to \infty} \frac{1}{2} \tau L \langle J_\tau([\eta])^2 \rangle^\text{st}_{E=0}.
\]

(39)
Then, the Green-Kubo relation connects the conductivity, $\sigma$, with the current fluctuation, $B$, by
\[ \sigma = \frac{B}{T}. \] (40)

**Proof:** We prove (40) using a rather special situation. Suppose that the statistical distribution of the configuration $\eta$ at $t = 0$ is canonical, $p^{\text{can}}(\eta)$, and the driving force $E$ is turned on at $t = 0$. In this transient process, the probability of a history $[\eta]$ is given by
\[ P_{t_{\text{E}}}^{\text{tr}}([\eta]) = p^{\text{can}}(\eta(0)) T(\eta(0) \to \eta(1)) \cdots T(\eta(LT - 1) \to \eta(L_T)). \] (41)

Then, from (29), (30) and (38), we can derive
\[ \frac{P_{t_{\text{E}}}^{\text{tr}}([\eta])}{P_{t_{\text{E}}}^{\text{tr}}(\tilde{[}\eta])} = e^{\beta E_T L J_{\tau}([\eta])}, \] (42)
where $\tilde{[}\eta]$ represents the time reversed history $(\eta(L_T), \eta(L_T - 1), \cdots, \eta(0))$.

Because the statistical average of a history dependent quantity $A$ by the probability $P_{t_{\text{E}}}^{\text{tr}}([\eta])$ is written as
\[ \langle A \rangle_{t_{\text{E}}}^{\text{tr}} \equiv \sum_{[\eta]} P_{t_{\text{E}}}^{\text{tr}}([\eta]) A([\eta]), \] (43)
the following identity is derived, using (42):
\[ \langle A \rangle_{t_{\text{E}}}^{\text{tr}} = \sum_{[\eta]} e^{\beta E_T L J_{\tau}([\eta])} P_{t_{\text{E}}}^{\text{tr}}(\tilde{[}\eta]) A([\eta]), \]
\[ = \sum_{[\eta]} e^{-\beta E_T L J_{\tau}([\eta])} P_{t_{\text{E}}}^{\text{tr}}([\eta]) \tilde{A}([\eta]), \]
\[ = \langle e^{-\beta E_T L J_{\tau}} \tilde{A} \rangle_{t_{\text{E}}}^{\text{tr}}, \] (44)
where $\tilde{A}([\eta]) \equiv A(\tilde{[}\eta])$, and we have used $J_{\tau}([\eta]) = -J_{\tau}([\eta])$ in deriving the second line. The expression (44) is the key identity to derive the universal relations in linear response theory. We emphasize that this key identity results from the local detailed balance condition (30) and that this identity is valid even outside the linear response regime.

Here, Setting $A = J_{\tau}$ in (44), we obtain
\[ \langle J_{\tau} \rangle_{t_{\text{E}}}^{\text{tr}} = \frac{1}{2} \langle (1 - e^{-\beta E_T L J_{\tau}}) J_{\tau} \rangle_{t_{\text{E}}}^{\text{tr}}, \] (45)
which is called the nonlinear response relation. Yamada and Kawasaki initially derived it [25] and then Kawasaki and Gunton generalized it [26]. Finally, by
expanding the right hand side of (45) with respect to $E$, (45) becomes

$$\bar{J} = \frac{B}{T} E + O(E^2),$$

where in the large $\tau$ limit, the statistical average in this special situation $\langle \rangle^\text{tr}_E$, is equal to the average in the steady state $\langle \rangle^\text{st}_E$. This expression provides (40) when the limit $E \to 0$ is used.

**Remark:** One may note that a long time tail of current fluctuation yields an anomalous contribution to the Green-Kubo relation. This long time tail is mainly due to momentum conservation [27]. In the one-dimensional driven lattice gas, the numerical check indicates that the long time tail of the current fluctuation only appear when $E \neq 0$. (See Refs. [28,29] for the case $E \neq 0$.) We conjecture that mode coupling effects are vanishing when $E = 0$, due to the absence of the momentum degrees of freedom. Thus, we cannot discuss a compatibility of the long time tail with the Green-Kubo relation within the one-dimensional lattice gas. However, it is generally understood that a long time tail does not cause the Green-Kubo relation to breakdown when we take a long time limit with a fixed system size [30].

### 4.2 Steady state distribution

We can show that the key identity (44) yields several relations by substituting the appropriate quantities into $A$. Through understanding of the fluctuation theorem, originally discovered in Ref. [31], the importance of (44) has been recognized [32,33,34,35]. Indeed, by setting $A([\eta]) = \delta(E\tau L J_r ([\eta]) - a)$, and by setting $A([\eta]) = 1$ in (44), we obtain the fluctuation theorem. It is noteworthy that the connection of the fluctuation theorem with the nonlinear response relation (45), which is also derived from (44), was noted by Crooks [35].

Furthermore, as indicated in Ref. [35], setting $A([\eta]) = \delta(\eta - \eta(\tau))$ in the key identity (44), the steady state distribution function is obtained as

$$p^\text{st}_E(\eta) = \lim_{\tau \to \infty} \langle e^{-\beta E\tau L J_r} \delta(\eta - \eta(0)) \rangle^\text{tr}_E,$$

(47) can be rewritten so that the deviation from the equilibrium distribution function, $p^\text{can}(\eta)$, is explicit. That is,

$$p^\text{st}_E(\eta) = p^\text{can}(\eta) \lim_{\tau \to \infty} \langle e^{-\beta E\tau L J_r} \rangle_{E, \eta(0) = \eta},$$

(48)

where $\langle \rangle_{E, \eta(0) = \eta}$ represents the average with the initial condition of $\eta(0) = \eta$.
when $t = 0$. Here, (48) can be also rewritten as

$$p_{st}^E(\eta) = p_{can}^{\eta}(\eta) \lim_{\tau \to \infty} e^{\sum_{n=1}^{\infty} \frac{1}{n!} (-\beta E \tau L)^n \langle (J_{\tau})^n \rangle_{E,\eta(0)=\eta}}, \quad (49)$$

where $\langle \cdot \rangle_{E,\eta(0)=\eta}$ denotes the cumulant. It should be noted that the expressions of the steady state distribution (48) and (49) are valid even outside the linear response regime.

Particularly, in the linear response regime, (49) is reduced to

$$p_{st}^E(\eta) = p_{can}^{\eta}(\eta) \lim_{\tau \to \infty} e^{-\beta E \tau L \langle J_{\tau} \rangle_{E=0,\eta(0)=\eta} + O(E^2)}.$$

This expression indicates that the deviation of $p_{st}^E(\eta)$ from the equilibrium distribution, $p_{can}^{\eta}(\eta)$, is represented by an entropy production. Zubarev and McLennan found a similar expression by studying the nonequilibrium steady state distribution [36,37].

Furthermore, when the contribution of the order $E^2$ is considered, $p_{st}^E(\eta)$ can be expressed as

$$p_{st}^E(\eta) = p_{can}^{\eta}(\eta) \lim_{\tau \to \infty} e^{-\beta E \tau L \langle J_{\tau} \rangle_{E=0,\eta(0)=\eta} + \frac{1}{2} (\beta E \tau L)^2 \langle (J_{\tau})^2 \rangle_{E=0,\eta(0)=\eta} + O(E^3)}.$$

It is interesting to see the fact that the existence of the Green-Kubo relation guarantees the convergence of the right-hand side of the expression (51) with the limit $\tau \to \infty$.

4.3 Reciprocity relation

To simply demonstrate the reciprocity relation [38,39], let us consider a rather artificial model that consists of two types of particles labeled, (X) and (Y). (X) particles are driven by $E_1$ while (Y) by $E_2$. In this situation, $Q(\eta \to \eta')$ defined in (29) becomes

$$Q(\eta \to \eta') = H_0(\eta') - H_0(\eta) - E_1 \sum_{x=0}^{L-1} \Phi_x^X(\eta \to \eta') - E_2 \sum_{x=0}^{L-1} \Phi_x^Y(\eta \to \eta'), \quad (52)$$

where $\Phi_x^X$ and $\Phi_x^Y$ are the net numbers of particles labeled (X) and (Y) that hop from $x$ to $x + 1$ for the configuration change $\eta \to \eta'$, respectively. Then, we define the spatially averaged currents per one MCS at time $t$, $j^X(t)$ and $j^Y(t)$ as
\[ j^X(t) \equiv \frac{1}{L} \sum_{x=0}^{L-1} \sum_{k=0}^{L-1} \Phi^X_x(\eta(Lt + k) \rightarrow \eta(Lt + k + 1)), \quad (53) \]

\[ j^Y(t) \equiv \frac{1}{L} \sum_{x=0}^{L-1} \sum_{k=0}^{L-1} \Phi^Y_x(\eta(Lt + k) \rightarrow \eta(Lt + k + 1)). \quad (54) \]

Using (53) and (54), the \( \tau \)-averaged currents are defined as

\[ J^X_\tau(\eta) \equiv \frac{1}{\tau} \sum_{t=0}^{\tau-1} j^X(t), \quad (55) \]

\[ J^Y_\tau(\eta) \equiv \frac{1}{\tau} \sum_{t=0}^{\tau-1} j^Y(t). \quad (56) \]

When \( E_1 \neq 0 \) and \( E_2 = 0 \), we derive the key identity in this situation:

\[ \langle A \rangle_{E_1}^{tr} = \langle e^{-\beta E_1 \tau L J^X_\tau} A \rangle_{E_1}^{tr}. \quad (57) \]

Setting \( A = J^Y_\tau \) and expanding (57) with respect to \( E_1 \), we obtain

\[ \langle j^Y \rangle_{E_1=E_2=0}^{st} = \frac{1}{2} \beta E_1 \tau L \langle J^X_\tau J^Y_\tau \rangle_{E_1=0}^{st} + O(E_1^2). \quad (58) \]

Here, we define the conductivity, \( \sigma_{12} \), which characterizes the transportation of type (Y) particles caused by the driving force \( E_1 \) (only applied to type (X) particles), as

\[ \sigma_{12} \equiv \lim_{E_1 \to 0} \frac{1}{E_1} \langle j^Y \rangle_{E_1=E_2=0}^{st}. \quad (59) \]

Then, (58) can be rewritten as

\[ \sigma_{12} = \frac{1}{2} \beta \tau L \langle J^X_\tau J^Y_\tau \rangle_{E_1=0,E_2=0}^{st}. \quad (60) \]

Considering the opposite case, when \( E_2 \neq 0 \) and \( E_1 = 0 \), we define the conductivity, \( \sigma_{21} \), as

\[ \sigma_{21} \equiv \lim_{E_2 \to 0} \frac{1}{E_2} \langle j^X \rangle_{E_1=0,E_2=0}^{st}. \quad (61) \]

In a similar way as deriving (60), we can also derive

\[ \sigma_{21} = \frac{1}{2} \beta \tau L \langle J^Y_\tau J^X_\tau \rangle_{E_1=0,E_2=0}^{st}. \quad (62) \]

From the trivial identity

\[ \langle J^X_\tau J^Y_\tau \rangle_{E_1=0,E_2=0}^{st} = \langle J^Y_\tau J^X_\tau \rangle_{E_1=0,E_2=0}^{st}, \quad (63) \]
we obtain the reciprocity relation between the conductivities as

$$\sigma_{12} = \sigma_{21}. \quad (64)$$

5 Fluctuation-response relation

The fluctuation-response relation (or the fluctuation-dissipation relation) represents a relation that connects a time dependent response to a time dependent external force with a time-correlation function in equilibrium. There are two types of fluctuation-response relations. One, which is regarded as an extension of the Green-Kubo relation, is when the external force is a time-dependent driving force. The other is when the external force is generated from a time dependent potential and is regarded as an extension of the fluctuation relation that can be derived within equilibrium statistical mechanics.

5.1 Main claim (time-dependent driving force)

Let us consider the case that the strength of the driving force $E(t)$ changes at every MSC. When the strength is sufficiently weak, the time-dependent averaged current $\langle j(t) \rangle$ (with an initial condition given at $t = -\infty$) is expressed by

$$\langle j(t) \rangle = \sum_{s=0}^{\infty} R(s) E(t - s) + O(E^2), \quad (65)$$

where $R(s)$ is independent of $E$, and is called a response function. Note that, from the causality, $R(t) = 0$ for $t < 0$. In a special situation when the driving force $E$ is turned on at $t = 0$; that is, $E(t) = E(=\text{const.})$ for $t \geq 0$ and $E(t) = 0$ for $t < 0$, the relation (65) becomes

$$\langle j(t) \rangle_{tr}^E = E \sum_{s=0}^{t} R(s) + O(E^2). \quad (66)$$

On the other hand, setting $A = j(\tau - 1)$ in the key identity (44) and using $A = -j(0)$, we can derive

$$\langle j(\tau - 1) \rangle_{tr}^E = \beta E \sum_{s=0}^{\tau-1} \langle j(s)j(0) \rangle_{st}^{E=0} - \langle j(0) \rangle_{tr}^E + O(E^2). \quad (67)$$

In the case $\tau = 1$, this expression yields

$$\langle j(0) \rangle_{tr}^E = \frac{1}{2} \beta E \langle j(0)^2 \rangle_{st}^{E=0} + O(E^2). \quad (68)$$
Substituting this into (67), we obtain
\[
\langle j(\tau - 1) \rangle^\text{tr}_E = \beta E \sum_{s=0}^{\tau-1} \theta(s) \langle j(s)j(0) \rangle^\text{st}_{E=0} + O(E^2),
\]
(69)
where \( \theta(s) = 1 \) for \( s \geq 1 \), and \( \theta(0) = 1/2 \). When we compare (66) and (69), using the time correlation function
\[
C(t) \equiv \langle j(t)j(0) \rangle^\text{st}_{E=0},
\]
(70)
we find the relation for \( t \geq 0 \):
\[
\theta(t)C(t) = TR(t).
\]
(71)
(71) can be rewritten as
\[
C(t) = T(R(t) + R(-t))
\]
(72)
for all \( t \). The relation (72) is called the fluctuation-response relation, which is a dynamic extension of the Green-Kubo relation.

5.2 Main claim (time-dependent potential)

The relation between the time correlation function and the response function can also be derived when a perturbation potential function becomes time dependent. Specifically, let us consider a situation when a time-dependent potential
\[
V_x \equiv v(t) \sin \frac{2\pi x}{L}
\]
(73)
is applied to the system. That is, the equilibrium Hamiltonian (16) is modified as
\[
H_V(\eta, t) \equiv H_0(\eta) + \sum_{x=1}^{L} \eta_x V_x.
\]
(74)
Here, the amplitude of the density fluctuation with wavenumber \( 2\pi/L \) is
\[
\hat{\rho}(t) \equiv \sum_{x=1}^{L} \eta_x (Lt) \sin \frac{2\pi x}{L}.
\]
(75)
Using (75), we define the response function, \( R_\rho(t) \), by the relation
\[
\langle \hat{\rho}(t) \rangle = -\sum_{s=0}^{\infty} R_\rho(s) v(t - s) + O(\Delta^2),
\]
(76)
with the initial condition given at \( t = -\infty \). Note that \( \langle \hat{\rho}(t) \rangle \) denotes the average in the situation. \( R_\rho(t) = 0 \) for \( t < 0 \) due to the causality. Then, for
t \geq 0, we can derive the relation
\[ C_\rho(t) = TR_\rho(t), \quad (77) \]
where
\[ C_\rho(t) \equiv \frac{1}{2} \langle (\hat{\rho}(t) - \hat{\rho}(0))^2 \rangle_{E=0}^{\text{st}}. \quad (78) \]
The relation (77) is also called the fluctuation-response relation.

We provide the proof of (77) using a special situation
\[ v(t) = \Delta \quad \text{for} \quad t \geq 0, \]
\[ = 0 \quad \text{for} \quad t < 0. \quad (79) \]
In this case, the relation (77) is explicitly rewritten as
\[ \langle \hat{\rho}(t) - \hat{\rho}(0) \rangle_{V}^{\text{tr}} = -\frac{\Delta}{2T} \langle (\hat{\rho}(t) - \hat{\rho}(0))^2 \rangle_{E=0}^{\text{st}} + O(\Delta^2), \quad (80) \]
where \( \langle \rangle_{V}^{\text{tr}} \) denotes the statistical average by the canonical distribution of \( v = 0 \) at \( t = 0 \) and by the transition probability \( T \) with \( v = \Delta \) for \( t \geq 0 \).
(Note that the canonical distribution is realized at \( t = 0 \), because the initial condition is given at \( t = -\infty \).) The form (80) can also be derived using a method similar to that used for the derivation of the Green-Kubo relation. Indeed, by repeating a procedure similar to those in Subsection 4.1, we can obtain the following key identity for an arbitrary history dependent quantity, \( A([\eta]) \):
\[ \langle A \rangle_{V}^{\text{tr}} = \langle e^{\beta \Delta (\hat{\rho}(t) - \hat{\rho}(0))} \tilde{A} \rangle_{V}^{\text{tr}}. \quad (81) \]
Setting \( A([\eta]) = \hat{\rho}(t) - \hat{\rho}(0) \) and expanding the right hand side with respect to \( \Delta \), we obtain (80).

Remark: Although (72) and (77) have similar forms, it should be noted that \( R_\rho \) does not represent the current response to the time-dependent potential perturbation. When we consider the current response to the time-dependent potential perturbation, we define the response function of the time difference of \( \hat{\rho} \), \( R_{\rho}^{\text{dl}}(t) \), by
\[ \langle \hat{\rho}(t + 1) - \hat{\rho}(t) \rangle = -\sum_{s=0}^{\infty} R_{\rho}^{\text{dl}}(s) \Delta(t - s) + O(\Delta^2). \quad (82) \]
Note that the time difference of \( \hat{\rho} \) is related to the current due to the continuum equation of the density field. Using the response function, \( R_{\rho}^{\text{dl}}(t) \), the relation (77) can be written as
\[ C_\rho(t + 1) - C_\rho(t) = T R_{\rho}^{\text{dl}}(t). \quad (83) \]
Remark 2: In addition to the proof using the key identity (81), which is directly due to the local detailed balance condition, there is another method to prove (80) [40]. Let $p_V^{\text{can}}(\eta)$ be the canonical distribution of the system with the perturbation $V_x$ of $v(t) = \Delta$. It is easy to find
\[ p_V^{\text{can}}(\eta) = (1 - \beta \Delta \hat{\rho}) p^{\text{can}}(\eta) + O(\Delta^2). \] (84)
Using this, we obtain
\[
\langle \hat{\rho}(t) - \hat{\rho}(0) \rangle_{E=0,V}^{\text{st}} = \langle (\hat{\rho}(t) - \hat{\rho}(0)) (1 + \beta \Delta \hat{\rho}(0)) \rangle_{E=0,V}^{\text{st}} + O(\Delta^2)
= \beta \Delta \langle \hat{\rho}(t) \hat{\rho}(0) \rangle_{E,V=0}^{\text{st}} - \beta \Delta \langle \hat{\rho}^2 \rangle_{E,V=0}^{\text{st}} + O(\Delta^2). \] (85)
(85) is equivalent to (80). In this method, we only use the condition that the stationary distribution of the system with the potential modulation is written as the canonical distribution. It means that (80) can be derived without using the local detailed balance condition, unlike the case of the Green-Kubo relation.

5.3 Fluctuation relation

When the limit $t \to \infty$ is taken, (80) becomes
\[
\langle \hat{\rho} \rangle_{E=0,V}^{\text{st}} = -\frac{\Delta}{T} \langle \hat{\rho}^2 \rangle_{E=0,V=0}^{\text{st}} + O(\Delta^2). \] (86)
As shown in the above proof (Remark 2), this kind of relation generally holds due to equilibrium statistical mechanics. The fluctuation-response relation (80) is a dynamic extension of this relation.

Here, we emphasize that (86) can be understood from a thermodynamic point of view. When $L$ is sufficiently large, $V_x$ of $v(t) = \Delta$ defined by (73), slowly varies in $x$. Thus, $V_x$ and $\langle \eta_x \rangle_{E=0,V}$ are regarded as smooth functions $V(x)$ and $\rho(x)$. Then, from a thermodynamic variational principle and using the free energy density for the equilibrium lattice gas, $f(T, \rho)$, the most probable density profile $\rho(x)$ under the influence of the slowly varying potential $V(x)$ is obtained as the minimizer of the functional
\[
F(\{\phi(x)\}) = \int_0^L dx [f(T, \phi(x)) + V(x)\phi(x)], \] (87)
under the constraint condition
\[
\int_0^L dx \phi(x) = L\rho. \] (88)
From this variational principle, $\rho(x)$ is determined so as to satisfy
\[ \mu(T, \rho(x)) + V(x) - \lambda = 0, \quad (89) \]
where $\lambda$ is the Lagrange multiplier due to the constraint condition, and $\mu(T, \rho)$ is the chemical potential defined by
\[ \mu \equiv \frac{\partial f(T, \rho)}{\partial \rho}. \quad (90) \]

Differentiating the relation (89) with respect to $x$, we obtain
\[ \frac{d\rho(x)}{dx} \left. \frac{\partial \mu(T, \rho)}{\partial \rho} \right|_{\rho=\rho(x)} + \frac{dV(x)}{dx} = 0. \quad (91) \]

Substituting (73) into (91), and using (75), we derive
\[ \langle \hat{\rho} \rangle_{E,V}^{\text{st}} = -\frac{L}{2} \left( \frac{\partial \mu(T, \bar{\rho})}{\partial \bar{\rho}} \right)^{-1} + O(\Delta^2), \quad (92) \]
where $\bar{\rho}$ is the averaged density.

Now, let us recall that the thermodynamic variational principle is derived from the Einstein-Boltzmann formula for the probability of the density profile:
\[ \text{Prob}(\{\rho(x)\}) \simeq \frac{\delta}{(\int_0^L dx(\rho(x) - \bar{\rho}))} e^{-\beta F(\{\rho(x)\})}. \quad (93) \]

When $V(x) = 0$, setting $\rho(x) = \bar{\rho} + \delta \rho(x)$ and expanding $f(T, \rho(x))$ with respect to $\delta \rho(x)$, we obtain
\[ \text{Prob}(\{\delta \rho(x)\}) \simeq \delta \left( \int_0^L dx \delta \rho(x) \right) e^{-\beta \left( \frac{\partial \mu(T, \bar{\rho})}{\partial \bar{\rho}} \right) \int_0^L dx (\delta \rho(x))^2}, \quad (94) \]
using the definition of the chemical potential (90). The expression (94) leads to the fluctuation relation
\[ \left( \frac{\partial \mu(T, \bar{\rho})}{\partial \bar{\rho}} \right)^{-1} = \frac{\chi_T}{T}, \quad (95) \]
where $\chi$ is the intensity of density fluctuations defined by
\[ \chi \equiv \Delta x \langle (\delta \rho(x))^2 \rangle_{E=0}^{\text{st}} \quad (96) \]
in the continuum description. Here, $\Delta x$ is the length much longer than the microscopic correlation length, but much shorter than the system size. $\rho(x)$ represents the coarse-grained density over the region of the length $\Delta x$.  

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Substituting this result into (92), we obtain

$$\langle \hat{\rho} \rangle_{E=0,V}^{st} = -\frac{L\Delta}{2T} \chi + O(\Delta^2). \quad (97)$$

Thus, (86) is the fluctuation relation, if we can prove the relation

$$\chi = \lim_{L \to \infty} \frac{2}{L} \langle (\hat{\rho} - \bar{\rho})^2 \rangle_{E=0}^{st}. \quad (98)$$

**Proof of (98):** Let us define the intensity of the density fluctuations $\chi$ more explicitly than that in the continuum description given in (96). Consider a coarse-grained density of the subsystem with the size $\ell$:

$$\rho_\ell \equiv \frac{1}{\ell} \sum_{x=1}^{\ell} \eta_x. \quad (99)$$

Then, using the quantity

$$d_{\ell,L} \equiv \ell \langle (\rho_\ell - \bar{\rho})^2 \rangle_{E=0}^{st}, \quad (100)$$

the intensity of density fluctuations, $\chi$, should be defined as

$$\chi \equiv \lim_{\ell \to \infty} \lim_{L/\ell \to \infty} d_{\ell,L}. \quad (101)$$

Based on this definition, we now derive (98). Notice the asymptotic relation

$$d_{\ell,L} \simeq \chi \frac{L - \ell}{L} \quad (102)$$

for $1 \ll \ell \ll L$. The derivation of (102) is explained as follows.

Let $N_\ell = \rho_\ell \ell$ and $\bar{N}_\ell = \bar{\rho} \ell$. Then, according to the central limit theorem, the probability of $N_\ell$ approaches to the form

$$\text{Prob}(N_\ell) \simeq e^{-\frac{(N_\ell - \bar{N}_\ell)^2}{2\chi\ell}} \frac{1}{2\chi(L-\ell)} \quad (103)$$

when $\ell$ and $L - \ell$ become large. From this, the probability of $\rho_\ell$ is written as

$$\text{Prob}(\rho_\ell) \simeq e^{-\frac{\ell L (\rho_\ell - \bar{\rho})^2}{2\chi(L-\ell)}}. \quad (104)$$

This implies (102).
Using this asymptotic relation, we obtain

$$\chi = 2 \lim_{L \to \infty} \frac{d_{L/2,L}}{L}. \tag{105}$$

Furthermore, we can derive

$$\lim_{L \to \infty} \frac{d_{L/2,L}}{L} = \lim_{L \to \infty} L \langle \hat{\rho}^2 \rangle_{E=0}^{st}, \tag{106}$$

using a straightforward calculation. Combining (105) and (106), we obtain the expression (98).

6 Einstein relation

As is well-known, one of the celebrated papers written by Einstein in 1905 is regarded as genesis of linear response theory [41,42]. Even in many-body systems, if a diffusion constant can be properly defined, it is connected with the conductivity in an extended form of the original Einstein relation for one-body systems. In this section, we derive the Einstein relation for the one-dimensional driven lattice gas. We also explain the interrelations among the Green-Kubo relation, the fluctuation-response relations, and the Einstein relation. At the end of this section, we discuss the Einstein relation from the thermodynamic point of view.

6.1 Main claim

We begin by defining the density diffusion constant, $D$. We first assume that the most probable process of the density field is described by a diffusion equation. On this assumption, $D$ should be defined as a coefficient of the diffusion term that appears in the equation. As an example, we consider the time evolution of the density field after the slowly varying weak potential is turned on at $t = 0$. When the most probable behavior in this situation can be described by the diffusion equation with the diffusion constant $D$, the response function $R_\rho(t)$, given in (76), can be expressed as

$$R_\rho(t) = R_\rho(\infty) \left( 1 - e^{-D(\frac{2\pi}{T})^2 t} \right). \tag{107}$$

In this paper, we assume that (107) determines the value of $D$.

Now, the Einstein relation in this model connects the diffusion constant, $D$, with the conductivity, $\sigma$, which is defined by (37), as

$$D\chi = \sigma T. \tag{108}$$
We derive (108) using both the Green-Kubo relation (40) and the fluctuation-response relation (80).

**Proof:** From (80) and (107), we obtain

$$
\langle (\hat{\rho}(t) - \hat{\rho}(0))^2 \rangle_{E=0}^{\text{st}} = 2 \langle \hat{\rho}^2 \rangle_{E=0}^{\text{st}} \left[ 1 - e^{-D(2\pi L)^2 t} \right].
$$

(109)

Notice the continuity equation

$$
\eta_x(Lt) - \eta_x(0) = -J_{x,t} + J_{x-1,t},
$$

(110)

with

$$
J_{x,t} \equiv \sum_{k=1}^{tL} \Phi_x(\eta(k-1) \rightarrow \eta(k)),
$$

(111)

where $\Phi_x(\eta \rightarrow \eta')$ is given in (28). Using (110) and (111), we derive

$$
\hat{\rho}(t) - \hat{\rho}(0) = \left( \frac{2\pi}{L} \right) \sum_{x=1}^{L} J_{x,t} \cos \frac{2\pi x}{L} + O \left( \frac{1}{L^2} \right).
$$

(112)

Next, we define

$$
B_\infty \equiv \lim_{t \to \infty} \lim_{L \to \infty} B_{1,t}(L)
$$

(113)

with

$$
B_{1,t}(L) \equiv \frac{1}{Lt} \left\langle \left( \sum_{x=0}^{L-1} J_{x,t} \cos \frac{2\pi x}{L} \right)^2 \right\rangle_{E=0}^{\text{st}},
$$

(114)

where the order of the two limits in (113) must not be exchanged. Then, from (98), (109) and (112), we find

$$
B_\infty = D \lim_{L \to \infty} \frac{2}{L} \langle \hat{\rho}^2 \rangle_{E=0}^{\text{st}} = D\chi.
$$

(115)

Furthermore, we can derive $B_\infty = B$ because the $\langle J_{x,t} J_{y,t} \rangle_{E=0}^{\text{st}}$ is a rapidly decaying function of $|x - y|$ ($\ll L/2$) at a fixed $t$. Thus, we obtain

$$
B = D\chi.
$$

(116)

Combining this relation with the Green-Kubo relation (40), we arrive at the Einstein relation (108).

**Remark:** We comment on the diffusion of a marked particle which is characterized by a tracer diffusion constant. The tracer diffusion constant is not equal to the bulk diffusion constant, $D$, represented by (107), and it is not related to the other quantities presented in this paper.
6.2 Interrelation

We argue the interrelations among the Green-Kubo relation (40), the fluctuation-response relation (80), and the Einstein relation (108). To simplify the argument, we assume that the time correlation function, $C_{\rho}(t)$, is written in an exponential form as a function of time. That is,

$$\langle (\hat{\rho}(t) - \hat{\rho}(0))^2 \rangle_{E=0}^{\text{st}} = 2 \langle \hat{\rho}^2 \rangle_{E=0}^{\text{st}} \left[ 1 - e^{-D_c \left( \frac{2\pi}{L} \right)^2 t} \right]. \tag{117}$$

Based on this assumption, the fluctuation-response relation (80) in the simple form is

$$D_c = D. \tag{118}$$

Similar to the derivation of (115), we can derive

$$B = D_c \chi \tag{119}$$

from the continuity equation. Now, when the fluctuation-response relation in the form (118) is valid, we find with the aid of (119) that the Green-Kubo relation (40) and the Einstein relation (108) are equivalent. Also, when both the relations (40) and (108) are valid, we obtain the fluctuation-response relation (118) by using (119). In this way, we have confirmed that any two of the three relations lead to the other relation, when $R_{\rho}(t)$ and $C_{\rho}(t)$ have the exponentially decaying forms.

For the driven lattice gas, using the diffusion constant, $D_c$, given in (117), Katz et al presented the rigorous proofs of the Green-Kubo relation and the Einstein relation [21] (although in a less systematic way than that presented here). It should be noted that there is the fluctuation-response relation (118) behind the adoption of this definition of the diffusion constant. Related to this issue, it is problematic in a system far from equilibrium whether to define the diffusion constant from a response function or a time correlation function, because for the one-dimensional driven lattice gas, the fluctuation-response relation (77) is violated in the nonequilibrium steady states [9].

Below, we demonstrate another important interrelation; the Einstein relation is equivalent to the thermodynamic fluctuation relation (95), when the relaxation of the density field is described more phenomenologically instead of using (107).

Let $\bar{J}(\rho, E)$ be the averaged particle current in a system with density $\rho$ and driving force $E$. When the slowly varying potential $V_x$ of $v(t) = \Delta$, given in (73), is applied to the system of $E = 0$, first the current should become $\bar{J}(\langle \eta_x \rangle_{E=0, V}^{\text{st}}, -dV_x/dx)$. Consequently, a diffusive current $D \langle (\eta_{x+1} - \eta_x) \rangle_{E=0, V}^{\text{st}}$
should appear so that the total current is equal to zero. That is,

\[ \bar{J}(\langle \eta_x \rangle_{E=0,V}^\text{st}, \frac{dV_x}{dx}) - D \langle (\eta_{x+1} - \eta_x) \rangle_{E=0,V}^\text{st} = 0. \] (120)

Precisely speaking, this relation is assumed to define \( D \) phenomenologically. As explained in Section 5, \( \langle \eta_x \rangle_{E=0,V}^\text{st} \) and \( V_x \) can be regarded as \( \rho(x) \) and \( V(x) \). Thus, (120) can be rewritten as

\[ \bar{J}(\rho, -\frac{dV}{dx}) - D \frac{d\rho}{dx} = 0. \] (121)

The expansion of (121) with respect to \( dV/dx \) yields

\[ -\sigma \frac{dV}{dx} - D \frac{d\rho}{dx} = 0. \] (122)

Note that \( |dV/dx| \) is sufficiently small because \( V(x) \) slowly varies in \( x \). Substituting the result of the thermodynamic variational principle (89) into (122), we obtain

\[ \sigma \frac{\partial \mu(T, \rho)}{\partial \rho} - D = 0. \] (123)

Then, the thermodynamic fluctuation relation (95) leads to the Einstein relation (108).

The above argument states that the non-triviality of the Einstein relation depends on the selection of which \( D \) to use among (107), (117) and (121). Also, it is amazing to see that the thermodynamic variational principle, the thermodynamic fluctuation relation, and linear response theory are mutually related.

Here, let us recall that the fluctuation-response relation (77) can be derived without the local detailed balance condition, but only if a general Markov process compatible with the statistical mechanics is used. Using this fact, and admitting the phenomenological derivation of the Einstein relation, we can derive the Green-Kubo relation. It implies that all the relations in linear response theory can be understood without the local detailed balance condition. Although the argument is correct, it assumes that the density field obeys a linear diffusion equation. We wish to emphasize that the Green-Kubo relation and the fluctuation-response relation are derived using the local detailed balance condition even when the density field does not obey a simple linear equation.
7 Green-Kubo relation in the boundary-driven lattice gas

In this section, we study a different type of nonequilibrium lattice gases where the particles are not driven by an external driving force in the bulk, but are driven by the difference in chemical potential between two particle reservoirs in contact with the boundaries. Due to the local detailed balance condition imposed on the model, we can derive the Green-Kubo relation in a boundary-driven lattice gas.

7.1 One-dimensional boundary-driven lattice gas

Consider the system in which the sites \( x = 1 \) and \( x = L \) are in contact with the particle reservoirs that have the chemical potentials \( \mu_1 \) and \( \mu_L \). Specifically, we set \( \mu_1 = \mu \) and \( \mu_L = \mu + \Delta \mu \). When \( \Delta \mu \neq 0 \), the particles flow in one direction on average, but when \( \Delta \mu = 0 \), the grand-canonical distribution is realized.

We describe the time evolution of the configuration of the system, \( \eta \), by iterating the following three Monte Carlo steps:

In the first step, a particle is created and annihilated at the site \( x = 1 \). This process is represented by flipping the value of \( \eta_1 \) with the probability \( c_1(\eta) \). Here, changing from \( \eta_1 = 0 \) to \( \eta_1 = 1 \) corresponds to creating a particle, while changing from \( \eta_1 = 1 \) to \( \eta_1 = 0 \) corresponds to annihilating a particle. The flipping probability, \( c_1(\eta) \), must satisfy the condition, which is a simple extension of (17),

\[
c_1(\eta) = c_1(\eta^1) e^{-\beta[H_0(\eta^1) - H_0(\eta) - \mu_1((\eta^1)_1 - \eta_1)]},
\]

(124)

where \( H_0(\eta) \) represents the interaction between particles, and its form is given by (16). Recall that \( \eta^1 \) denotes the configuration of the system after flipping the value of \( \eta_1 \) (see Section 3 for the usage). Logically speaking, the condition (124) is necessary for the transition probability to satisfy the local detailed balance condition in nonequilibrium steady states. We will check this condition in the next subsection.

In the second step, we provide a time evolution rule for the bulk. We randomly select a nearest neighbor pair \( x, y \), and exchange the value of \( \eta_x \) and \( \eta_y \) with the probability \( c_{\text{bulk}}(x, y; \eta) \) to satisfy

\[
c_{\text{bulk}}(x, y; \eta) = c_{\text{bulk}}(x, y; \eta^{xy}) e^{-\beta[H_0(\eta^{xy}) - H_0(\eta)]}.
\]

(125)

We also define \( c_{\text{bulk}}(x, y; \eta) = 0 \) for \( |x - y| \neq 1 \). Note that this process is the same as that for the lattice gas without the particle reservoirs.
In the third step, the procedure of the first step is performed at the site \( x = L \). That is, we change the value of \( \eta_L \) to that of \( 1 - \eta_L \) with the probability \( c_L(\eta) \) to satisfy

\[
c_L(\eta) = c_L(\eta') e^{-\beta [H_0(\eta') - H_0(\eta) - \mu_L((\eta')_L - \eta_L)]}.
\] (126)

Then, the corresponding transition probabilities \( T_1(\eta \rightarrow \eta') \), \( T_{\text{bulk}}(\eta \rightarrow \eta') \) and, \( T_L(\eta \rightarrow \eta') \) are defined as

\[
T_1(\eta \rightarrow \eta') = c_1(\eta) \quad \text{for} \quad \eta' = \eta^1 \neq \eta, \tag{127}
\]
\[
T_{\text{bulk}}(\eta \rightarrow \eta') = \frac{1}{L-1} c_{\text{bulk}}(x, y; \eta) \quad \text{for} \quad \eta' = \eta^xy \neq \eta, \tag{128}
\]
\[
T_L(\eta \rightarrow \eta') = c_L(\eta) \quad \text{for} \quad \eta' = \eta^L \neq \eta. \tag{129}
\]

The transition probabilities \( T_1(\eta \rightarrow \eta) \), \( T_{\text{bulk}}(\eta \rightarrow \eta) \), and \( T_L(\eta \rightarrow \eta) \) are determined from the normalization conditions of the probability

\[
\sum_{\eta'} T_1(\eta \rightarrow \eta') = 1, \tag{130}
\]
\[
\sum_{\eta'} T_{\text{bulk}}(\eta \rightarrow \eta') = 1, \tag{131}
\]
\[
\sum_{\eta'} T_L(\eta \rightarrow \eta') = 1, \tag{132}
\]

respectively. Notice that these expressions of the transition probabilities lead to the equalities

\[
\frac{T_1(\eta \rightarrow \eta')}{T_1(\eta' \rightarrow \eta)} = e^{-\beta [H_0(\eta') - H_0(\eta) - \mu_1((\eta')_1 - \eta_1)]}, \tag{133}
\]
\[
\frac{T_{\text{bulk}}(\eta \rightarrow \eta')}{T_{\text{bulk}}(\eta' \rightarrow \eta)} = e^{-\beta [H_0(\eta') - H_0(\eta)]}, \tag{134}
\]
\[
\frac{T_L(\eta \rightarrow \eta')}{T_L(\eta' \rightarrow \eta)} = e^{-\beta [H_0(\eta') - H_0(\eta) - \mu_L((\eta')_L - \eta_L)]}. \tag{135}
\]

7.2 Local detailed balance condition

Using the above time evolution rule, a history of configurations during \( \tau \) MCS is denoted as \([\eta] = (\eta(0), \eta(1), \cdots, \eta(3L\tau))\). For a segment of the history \([\eta]_k = (\eta(3k), \eta(3k + 1), \eta(3k + 2), \eta(3k + 3))\), where \( k = 0, 1, 2, \cdots, L\tau - 1 \), we define the product of the transition probability, \( T([\eta]_k) \), as
\[ T([\eta]_k) = T_1(\eta(3k) \to \eta(3k+1))T_{\text{bulk}}(\eta(3k+1) \to \eta(3k+2)) \times T_L(\eta(3k+2) \to \eta(3k+3)). \] (136)

Associated with \( T([\eta]_k) \), we also define

\[ T^*([\eta]_k) = T_1(\eta(3k) \to \eta(3k+1))T_{\text{bulk}}(\eta(3k+1) \to \eta(3k+2)) \times T_1(\eta(3k+2) \to \eta(3k+3)). \] (137)

The transition probability \( T^*([\eta]_k) \) corresponds to the time evolution rule obtained by exchanging the first and third steps introduced in the last subsection. Furthermore, \([\eta]^*_k = (\eta(3k+3), \eta(3k+2), \eta(3k+1), \eta(3k))\) represents the time reversed segment of \([\eta]_k\). Then, from (133), (134) and (135), we obtain the relation

\[ \frac{T([\eta]_k)}{T^*([\eta]_k)} = e^{-\beta[H_0(\eta(3k+3)) - H_0(\eta(3k)) - \mu_1 \Phi_1(k) - \mu_L \Phi_L(k)]}, \] (138)

where

\[ \Phi_1(k) \equiv \eta_1(3k+1) - \eta_1(3k), \] (139)

and

\[ \Phi_L(k) \equiv \eta_L(3k+3) - \eta_L(3k+2). \] (140)

\( \Phi_1(k) \) and \( \Phi_L(k) \) are numbers of particles that flow into the system from the particle reservoirs during the time steps from \( 3k \) to \( 3k+3 \) at \( x = 1 \) and at \( x = L \), respectively.

Now, the increment of the particle number at the site \( x \) from \( t = 3k+3 \) to \( t = 3k \) is

\[ \delta \eta_x(k) \equiv \eta_x(3k+3) - \eta_x(3k). \] (141)

Because the total particle number is conserved, the following relation holds:

\[ \sum_{x=1}^{L} \delta \eta_x(k) = \Phi_1(k) + \Phi_L(k). \] (142)

Using this relation, and recalling that \( \mu_1 = \mu \) and \( \mu_L = \mu + \Delta \mu \), the equality (138) can be rewritten as

\[
\begin{align*}
\frac{T([\eta]_k)}{T^*([\eta]_k^*)} &= e^{-\beta[H_0(\eta(3k+3)) - H_0(\eta(3k)) - \mu \sum_{x=1}^{L} \delta \eta_x(k) - \Delta \mu \Phi_L(k)]} \\
&= e^{-\beta[H_0(\eta(3k+3)) - \mu \sum_{x=1}^{L} \eta_x(3k+3) - H_0(\eta(3k)) - \mu \sum_{x=1}^{L} \eta_x(3k) - \Delta \mu \Phi_L(k)]}. \tag{143}
\end{align*}
\]

This is regarded as the local detailed balance condition in the boundary-driven lattice gas.

In the equilibrium case \( \Delta \mu = 0 \), (143) leads to

\[ p^{\text{can}}(\eta(3k))T([\eta]_k) = p^{\text{can}}(\eta(3k+3))T^*([\eta]_k^*), \] (144)
with the grand-canonical distribution $p^\text{gcan}(\eta)$

$$p^\text{gcan}(\eta) \equiv \frac{1}{Z} e^{-\beta[H_0(\eta) - \mu \sum_{x=1}^{L} \eta_x]}, \quad (145)$$

where $Z$ denotes the normalization factor. The equality (144) corresponds to the detailed balance condition with respect to the grand-canonical distribution. This ensures that (145) is the steady state distribution of the stochastic model.

### 7.3 Main claim

In order to derive the Green-Kubo relation in this model, we assume that the grand-canonical distribution $p^\text{gcan}(\eta)$ of the chemical potential $\mu$ is realized at $t = 0$. Then, we consider the situation where $\Delta \mu \neq 0$ when $t \geq 0$. In this case, the probability of a history $[\eta] = (\eta(0), \eta(1), \ldots, \eta(3L \tau))$ is given by

$$P^\text{tr}_\Delta(\eta) \equiv p^\text{gcan}(\eta(0))T(\eta_0) \cdots T(\eta_{L \tau - 1}). \quad (146)$$

The path probability associated with $T^*$ is also defined as

$$P^\text{tr}_\Delta^*(\eta) \equiv p^\text{gcan}(\eta(0))T^*(\eta_0^*) \cdots T^*(\eta_{L \tau - 1}^*). \quad (147)$$

Noting the equality

$$P^\text{tr}_\Delta^*(\tilde{\eta}) = p^\text{gcan}(\eta(L \tau))T^*(\eta_{L \tau - 1}^*) \cdots T^*(\eta_0^*), \quad (148)$$

and using the local detail balance condition (143), we obtain

$$\frac{P^\text{tr}_\Delta(\eta)}{P^\text{tr}_\Delta^*(\eta)} = e^{\beta \Delta \mu J_\tau(\eta)}, \quad (149)$$

with

$$J_\tau(\eta) \equiv \frac{1}{\tau} \sum_{k=0}^{L \tau - 1} \Phi_L(k). \quad (150)$$

Then, we write the statistical average in the transient process by the probability, $P^\text{tr}_\Delta(\eta)$, as

$$\langle A \rangle^\text{tr}_\Delta = \sum_{[\eta]} P^\text{tr}_\Delta(\eta) A(\eta), \quad (151)$$

for a history dependent quantity $A(\eta)$. $\langle A \rangle^\text{tr}_\Delta$ is also defined in the same way, replacing $P^\text{tr}_\Delta(\eta)$ by $P^\text{tr}_\Delta^*(\eta)$ in (151).

Noting the equality $J_\tau(\tilde{\eta}) = -J_\tau(\eta)$, we obtain the key identity
\[
\langle A \rangle^\text{tr}_{\Delta \mu} = \sum_{\eta} e^{\beta \Delta \mu \tau J_\tau(\eta)} P^\text{tr*}_{\Delta \mu}(\eta) A(\eta),
\]
\[
= \sum_{\eta} e^{-\beta \Delta \mu \tau J_\tau(\eta)} P^\text{tr*}_{\Delta \mu}(\eta) \tilde{A}(\eta),
\]
\[
= \langle e^{-\beta \Delta \mu \tau J_\tau(\eta)} \tilde{A} \rangle^\text{tr*}_{\Delta \mu},
\]
where we have defined \( \tilde{A}(\eta) = A(\tilde{\eta}) \).

Here, setting \( A = J_\tau \) in (152), taking the limit \( \tau \to \infty \) and expanding the right hand side of (152) with respect to \( \Delta \mu \), we can derive
\[
\langle J_\tau \rangle^\text{st}_{\Delta \mu} = \frac{B}{T} \Delta \mu + O(\Delta \mu^2),
\]
with
\[
B \equiv \lim_{\tau \to \infty} \tau^2 \left( \langle (J_\tau)^2 \rangle^\text{st}_{\Delta \mu=0} \right).
\]

Note that \( \langle J_\tau \rangle^\text{tr}_{\Delta \mu} \) and \( \langle J_\tau \rangle^\text{tr*}_{\Delta \mu} \) are equal to the average in the steady state \( \langle J_\tau \rangle^\text{st}_{\Delta \mu} \) with the large \( \tau \) limit and a fixed system size \( L \). The expression (153) provides the Green-Kubo relation in the boundary-driven lattice gas, because the current correlation \( B \) in the system under the equilibrium condition is related to the conductivity \( \sigma \) in the nonequilibrium in the form \( B = \sigma T \), where \( \sigma \) is defined as
\[
\sigma \equiv \lim_{\Delta \mu \to 0} \frac{\langle J_\tau \rangle^\text{st}_{\Delta \mu}}{\Delta \mu}.
\]

We remark that the other relations derived in Sections 5 and 6 can be obtained, using the local detailed balance condition (143). As far as we know, the Green-Kubo relation in this model was presented in a different manner in Ref. [20]. Our derivation method is more pedagogical in the sense that the role of the local detailed balance condition is explicit.

8 Discussion

We have derived the universal relations of linear response theory for bulk-driven and boundary-driven lattice gases in a simple manner. We have also elucidated the interrelations among these universal relations, statistical mechanics and thermodynamics. However, in the arguments presented above, some important topics related to linear response theory were not discussed. Among them, there are two that are particularly worth consideration, the derivation of the universal relations from classical or quantum systems, and the extension of the universal relations to forms valid in nonequilibrium steady states far from equilibrium. In this final section, we present remarks on these two topics.
8.1 Microscopic understanding

It is well known that the universal relations of linear response theory can be derived from a microscopic description in the following way. (i) The system under consideration is assumed to be in equilibrium at $t = -\infty$; that is, the distribution of microscopic variables is assumed to be canonical at $t = -\infty$. (ii) An external force is applied to the system under the assumption that the time evolution obeys the Liouville and von Neumann equations. This assumption implies that the system does not interact with other dynamical degrees of freedom. (iii) The statistical average of the quantity of interest at time $t$ is calculated perturbatively up to linear order in the applied external force.

Within such a framework, it is straightforward to derive the linear response relations, but it is difficult to understand the physical picture. For example, let us consider an electric conduction system. In such a system, energy is continuously introduced into the system when an electric field is applied. Thus, obviously, a steady state is never realized unless the system contact with a heat bath. Then, recalling the step (ii) described above in the previous paragraph, it can be claimed that the formal calculation is not performed based on the realization of nonequilibrium steady states, even if the desired formulas can be derived by this method.

Furthermore, it should be noted that the time correlation (e.g. current correlations) in the formal perturbation scheme is calculated by use of mechanical time evolution equations without identifying the degrees of freedom that constitute the heat bath. If the energy dissipation into the heat bath is taken into account when the time correlation is calculated, it is plausible that the result of the calculation would depend on the nature of the heat bath. Indeed, in the stochastic models studied in this paper, the functional form of the time correlation depends on the choice of the stochastic rule (e.g. (19), (20), and (21)), which represent the nature of the heat bath, though the validity of the universal relations is independent of this choice.

Considering these points, we find that we do not obtain a clear understanding of nonequilibrium systems, even in the linear response regime, when we study systems on the basis of a microscopic description. Here, let us recall our method of derivation for the universal relations in the stochastic models. In our derivations, the steady state is prepared from the outset, and all the relations can be obtained by use of the local detailed balance condition. Thus, focusing on the realization of nonequilibrium steady states and the local detailed balance condition, we suggest that the two problems described below should be studied in microscopic systems.

The first problem is to clarify the conditions under which a subsystem exhibit-
ing a nonequilibrium steady state is determined in a purely mechanical system despite a continuous injection of energy. (Note that a nonequilibrium system with a Gaussian thermostat [43] is not regarded as a purely mechanical system of the type we wish to study.) Then, we characterize the heat bath by studying the mechanism of the energy dissipation, but it is not certain that a simple characterization is possible. If we succeed in the proper characterization, the second problem is to demonstrate the validity of the local detailed balance condition for these states. Then, given the local detailed balance condition, it is straightforward to derive universal relations. In this way, through the present study, we have identified a new direction in the investigation of the nature of nonequilibrium systems on the basis of a microscopic description.

8.2 Extension of the linear response relations

One may wonder whether it is possible to extend linear response theory to systems far from equilibrium. A partial answer to this question is provided by the nonlinear response relation given in (44), which provides a starting point to connect transport properties of systems far from equilibrium with dynamical fluctuations. Indeed, when Kawasaki and Gunton derived an expression for the nonlinear shear viscosity from the Liouville equation, the nonlinear response formula [26], which takes essentially the same form as (44), played a key role.

There is another approach to the extension of the universal relations that does not involve nonlinear response theory. In this approach, instead of studying nonlinear transport properties, the linear response properties near nonequilibrium steady states are studied by applying small perturbations as probes. It is believed that there is a close relationship between the linear response properties and the dynamical fluctuation properties, although, obviously, the universal relations that hold within the linear response regime cannot be valid in general outside this regime. Unlike the nonlinear response theory represented by (44), this type of extension of the universal relations beyond the linear response regime has not yet been established.

As a preliminary step in the attempt to employ this second type of approach to construct an extension of the universal relations to systems far from equilibrium (i.e., outside the linear response regime), recently, numerical experiments on a two-dimensional driven lattice gas were performed [11]. According to the results of this study, with respect to the properties of the system along the direction transverse to the external driving force, the linear responses of the system to perturbation forces are related to the fluctuations in the same form as the linear response relations. Here, it is important to note that in the direction transverse to the external driving force, the thermodynamic free energy, from which we can obtain the probability distribution for density fluctuations,
was constructed using the Maxwell relation [44,45]. (The Maxwell relation is the integrability condition yielding the free energy.) We conjecture that the validity of the extended forms of the linear response relations [11] is related to the existence of the thermodynamic function constructed in Ref. [44], recalling the argument given in Section 6.

Although these numerical results for states far from equilibrium are interesting, our understanding of the extended relations remains poor. In particular, there are the following two serious problems. First, it is well known that long-range spatial correlations of density fluctuations exist in nonequilibrium systems of two or more dimensional [46,47,48]. These long-range correlations are inconsistent with the extensive nature of thermodynamic fluctuation theory. In fact, we do not understand how the numerical results of Ref. [11,44] can be reconciled with the existence of long-range correlations. (See Ref. [45] for a related discussion). Second, while we were able to numerically construct an extended free energy and confirm the validity of the extended linear response relations along the direction transverse to the external driving force, it seems more difficult to find similar relations along the direction parallel to the driving force. Indeed, the study of a one-dimensional driven lattice gas far from equilibrium has revealed that the relationship between the fluctuations and the response to a probe force is complicated, because the fluctuations take the influence of hydrodynamic effects [9].

In order to construct a self-contained theory of nonequilibrium steady states, we need a unified treatment of thermodynamic and hydrodynamic fluctuations. For example, thinking optimistically, despite the existence of the long-range spatial correlations in nonequilibrium steady states, it might be possible to extract the thermodynamic component of the fluctuations by separating out of the long-range component. At present, however, there is no theory providing such a treatment. However, we should mention that the additivity principle proposed in Refs. [49,50] might provide a useful tool to study this problem, because this principle provides an elegant method by which the thermodynamic part of density fluctuations can be distinguished from the hydrodynamic part. Although the validity of this principle has been confirmed only for certain exactly solvable nonequilibrium models, it would be interesting to consider its application to a wider class of nonequilibrium models and to study how thermodynamic fluctuations can be extracted by use of this additivity principle.

If we could construct a unified treatment of fluctuations for nonequilibrium steady states far from equilibrium, our next step would be to seek new universal relations between fluctuations and response properties to probe forces in such systems. In that pursuit, and in the construction of a general theory of nonequilibrium steady states, the present paper, in which we have elucidated the interrelations among the linear response relations, statistical mechanics and thermodynamics, should serve as a useful guide.
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References

[1] R. Kubo, M. Toda, N. Hashitsume, Statistical Physics II: Nonequilibrium
Statistical Mechanics, Springer, Berlin, 1991.
[2] G. Eyink, J. L. Lebowitz and H. Spohn, J. Stat. Phys. 83 (1996) 385.
[3] A. Crisanti and F. Ritort, J. Phys. A 36 (2003) R181.
[4] L. F. Cugliandolo, J. Kuchan, and L. Peliti, Phys. Rev. E 55 (1997) 3898.
[5] L. Berthier and J-L. Barrat, Phys. Rev. Lett. 89 (2002) 095702.
[6] I. K. Ono, C. S. O'Hern, D. J. Durian, S. A. Langer, A. J. Liu, and S. R. Nagel,
Phys. Rev. Lett. 89 (2002) 095703.
[7] A. B. Kolton, R. Exartier, L. F. Cugliandolo, D. Doméıgue, and N. Grønbech-Jensen,
Phys. Rev. Lett. 89 (2002) 227001.
[8] K. Hayashi and S. Sasa, Phys. Rev. E 69 (2004) 066119.
[9] K. Hayashi and S. Sasa, Phys. Rev. E 71 (2005) 046143.
[10] K. Hayashi and S. Sasa, Phys. Rev. E 71 (2005) 020102(R).
[11] K. Hayashi, Phys. Rev. E 72 (2005) 047105.
[12] T. Harada, K. Hayashi and S. Sasa, J. Phys. A: Math. Gen. 38 (2005) 3799-3812.
[13] T. Harada and K. Yoshikawa, Phys. Rev. E 69 (2004) 031113.
[14] T. Harada and S. Sasa, Phys. Rev. Lett. 95 (2005) 130602.
[15] M. S. Green, J. Chem. Phys. 22 (1954) 398.
[16] H. B. Callen and T. A. Welton, Phys. Rev. 83 (1951) 34.
[17] R. Kubo and K. Tomita, J. Phys. Soc. Jpn 9 (1954) 888.
[18] H. Nakano, Prog. Theor. Phys. 17 (1957) 145.
[19] R. Kubo, J. Phys. Soc. Jpn 12 (1957) 570.

[20] H. Spohn, Large Scale Dynamics of Interacting Particles, Springer-Verlag, 1991.

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

[22] B. Schmittman and R. K. P. Zia, Phase transitions and Critical Phenomena Volume 17, Statistical Mechanics of Driven Diffusive Systems, Academic Press, 1995.

[23] J. Marro and R. Dickman, Nonequilibrium Phase Transitions in Lattice Models, Cambridge University Press, 1999.

[24] K. Sekimoto, J. Phys. Soc. Jpn. 66 (1997) 1234.

[25] T. Yamada and K. Kawasaki, Prog. Theor. Phys. 38 (1967) 1031.

[26] K. Kawasaki and J. D. Gunton, Phys. Rev. A 8 (1973) 2048.

[27] Y. Pomeau and P. Résibois, Physics Report 19 (1975) 63.

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

[29] M. Prähofer and H. Spohn, J. Stat. Phys. 115 (2004) 255.

[30] T. Murakami, T. Shimada, S. Yukawa and N. Ito, J. Phys. Soc. Jpn. 72 (2003) 1049.

[31] D. J. Evans, E. G. D. Cohen, and G. P. Morris, Phys. Rev. Lett. 71 (1993) 2401.

[32] G. Gallavotti and E. G. D. Cohen, Phys. Rev. Lett. 74 (1995) 2694.

[33] J. Kurchan, J. Phys. A: Math. Gen. 31 (1998) 3719.

[34] C. Maes, J. Stat. Phys. 95 (1999) 367.

[35] G. E. Crooks, Phys. Rev. E 61 (2000) 2361.

[36] D. N. Zubarev, Nonequilibrium Statistical Thermodynamics, Consultants Bureau, New York, 1974.

[37] J. A. McLennan, Introduction to Nonequilibrium Statistical Mechanics, Prentice-Hall, Englewood Cliffs, New Jersey, 1989.

[38] L. Onsager, Phys. Rev. 37 (1931) 405.

[39] L. Onsager, Phys. Rev. 38 (1931) 2265.

[40] A. Yoshimori, private communication.

[41] A. Einstein, Ann. Phys. 17 (1905) 549.

[42] A. Einstein, Introduction on the Theory of Brownian Movement, Dover, New York, 1956.

[43] S. Nosé, Prog. Theor. Suppl. 103 (1991) 117.
[44] K. Hayashi and S. Sasa, Phy. Rev. E 68 (2003) 035104(R).

[45] S. Sasa and H. Tasaki, e-print, cond-mat/0411052 to appear in J. Stat. Phys.

[46] J. R. Dorfman, T. R. Kirkpatrick, J. V. Sengers, Annu. Rev. Phys. Chem. 45 (1994) 213.

[47] H. Tasaki, e-print, cond-mat/0407262

[48] S. Sasa, Physica D 205 (2005) 233.

[49] B. Derrida, J. L. Lebowitz, and E. R. Speer, Phys. Rev. Lett. 87 (2001) 150601.

[50] B. Derreda, J. L. Lebowitz, and E. R. Spear, Phys. Rev. Lett. 89 (2002) 030601.