# Thermodynamic relations in a driven lattice gas: Numerical experiments

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We explore thermodynamic relations in nonequilibrium steady states with numerical experiments on a driven lattice gas. After operationally defining the pressure and chemical potential in the driven lattice gas, we confirm numerically the validity of the integrability condition (the Maxwell relation) for the two quantities whose values differ from those for an equilibrium system. This implies that a free-energy function can be constructed for the nonequilibrium steady state that we consider. We also investigate a fluctuation relation associated with this free-energy function. Our result suggests that the compressibility can be expressed in terms of density fluctuations even in nonequilibrium steady states.

A rich variety of nonequilibrium phenomena have been successfully described by phenomenological evolution equations. However, the microscopic foundation of such equations has not yet been established, except for systems near equilibrium. Even for nonequilibrium steady states (NESS) realized in simple systems, such as those involving only heat conduction and shear flow, appropriate statistical measures of microscopic configurations are not known. Recalling that equilibrium statistical mechanics was constructed with the aid of thermodynamics, we expect that checking the validity of thermodynamic relations in NESS is an important step in constructing a theory of nonequilibrium statistical mechanics.

Nonequilibrium lattice gases are simple mathematical models which have been useful in the elucidation of universal properties of NESS [1]. Topics studied with such models include nonequilibrium phase transitions [2], long-range spatial correlations [3], fluctuation theorems [4], nonlocal large deviation functionals [5], as well as mathematical foundations of nonequilibrium statistical mechanics [6]. It is thus expected that the nonequilibrium lattice gases provide good models for the exploration of thermodynamic relations.

There have been some proposals of an extended thermodynamic framework applicable to NESS [7,8]. In one such study, Sasa and Tasaki start from operational definitions of the pressure $p$ and chemical potential $\mu$, and they derive from these a quantitative relation which can be tested experimentally [8]. Because the Maxwell relation for $p$ and $\mu$ plays an essential role in the derivation of this relation, we are led to study the same Maxwell relation in the case of a driven lattice gas.

In this paper, we present numerical results that confirm the validity of the Maxwell relation for $p$ and $\mu$, which we define operationally for the system we study. As we explain below, the Maxwell relation provides an integrability condition for $p$ and $\mu$, and this yields a free-energy function extended to the NESS that we consider. The existence of this free-energy function leads us to believe that there is an associated fluctuation relation. Indeed, our numerical experi-

ments suggest that the compressibility can be expressed in terms of density fluctuations even in certain nonequilibrium systems.

## MODEL

Let $\sigma_i$ be an occupation variable defined on each site $i = (i_x, i_y)$ in a two-dimensional square lattice $\{(i_x, i_y) | 0 \leq i_x \leq L+1, 0 \leq i_y \leq M+1\}$. The variable $\sigma_i$ is 1 when the $i$th site is occupied and is 0 if it is empty. We assume periodic boundary conditions in the $x$ direction [i.e., $\sigma_i = \sigma_j$ when when $i = j + (L, 0)$] and no-flux boundary conditions in the $y$ direction (i.e., $\sigma_i = 0$ when $i_y = 0, M+1$). The array of all occupation variables $\{\sigma_i\}$ is denoted as $\sigma$ and called the "configuration."

We study a driven lattice gas with the Hamiltonian

$$H(\sigma) = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j - E \sum_i i_x \sigma_i, \qquad (1)$$

where $\langle i, j \rangle$ represents a nearest neighbor pair and $E$ is an external force [2]. The time evolution of $\sigma$ is described by the following rule: At each time step, we choose randomly a nearest neighbor pair $\langle i, j \rangle$, and exchange the values of $\sigma_i$ and $\sigma_j$ with the probability $c(i, j; \sigma)$ given by

$$c(i,j;\sigma) = \frac{1}{1 + \exp\{\beta[H(\sigma^{ij}) - H(\sigma)]\}}, \qquad (2)$$

where $\sigma^{ij}$ is the configuration obtained from $\sigma$ through this exchange and $\beta$ is the inverse temperature [9]. This exchange probability is called the heat bath method and is one of the most standard update rules satisfying the local detailed balance condition, the condition which is regarded to be natural in physical systems. The particle number $N = \Sigma_i \sigma_i$ is conserved throughout the time evolution. In this study, we fix $\beta = 0.5$, in which case the system is far from critical in the high temperature region.

## PRESSURE

In the equilibrium case ($E = 0$), the pressure is calculated by using equilibrium statistical mechanics. However, be-

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cause we do not know the proper statistical measure in NESS, in this case we should define the pressure in an operational manner. Although the pressure is usually defined as the normal force exerted on a unit area of a surface, there is no quantity corresponding to the force in a lattice gas. We thus define the pressure in terms of the quasistatic work required to change the system size. In order to allow for the calculation of this quantity in our lattice gas [10], we add a wall potential to the Hamiltonian $H(\sigma)$ in the form

$$H_w(\sigma) = H(\sigma) + \sum_{i:i_y=M} \sigma_i w. \qquad (3)$$

Because of the boundary conditions we impose, no particle can exist at sites with $i_y = M+1$, and therefore the system size in the $y$ direction is $M$. Now, according to Eq. (3), as $w$ is increased, it becomes increasingly unlikely for particles to exist at sites with $i_y = M$. When $w$ becomes sufficiently large, the average occupation number for sites with $i_y = M$ can be considered zero. We denote the value of $w$ beyond which this is the case as $w_m$. Hence, in the process that $w$ changes from 0 to $w_m$, the effective system size in the $y$ direction changes from $M$ to $M-1$. The quasistatic work performed to the system through this process is interpreted as the pressure multiplied by $L$. That is, the pressure $p$ is written as

$$p = \lim_{w_m \to \infty} \frac{1}{L} \int_0^{w_m} dw \sum_\sigma P^w_{N,M}(\sigma) \frac{\partial H_w(\sigma)}{\partial w}, \qquad (4)$$

where $P^w_{N,M}$ is the steady state distribution for a given value of $w$. It is easily proved that this definition of the pressure is equivalent to statistical mechanical formula in equilibrium.

In the numerical experiments, values of $p$ are obtained in the following way. Starting from random initial conditions, we carry out the time evolution with $w=0$ for a sufficiently long time, say $t_0$. In this way, we obtain a steady state with $w=0$. Next, we increase the value of $w$ by a quantity $\Delta w$ per Monte Carlo step per site (mcs) until $w$ reaches $w_m$. Then, noting that $\partial H_w(\sigma)/\partial w = \sum_{i:i_y=M} \sigma_i$, we measure the value of $\sum_{i:i_y=M} \sigma_i$ as $n(t)$ at time $t$, where zero of the time is defined as the point at which $w$ starts to increase. In one process from $w=0$ to $w=w_m$, we calculate

$$p = \frac{\Delta w}{L} \sum_{t=1}^{t_m} n(t), \qquad (5)$$

where $t_m$ is the time at which $w=w_m$. Then, determining carefully how the statistical distribution of $p$ depends on $w_m$ and $\Delta w$, we estimate the value of $p$ in the limit $w_m \to \infty$, $\Delta w \to 0$ [11].

In Fig. 1, we display an example of measured values of the pressure for densities in systems with $E=0$ and $E=10$. It is important to note that our analysis is not restricted to systems near equilibrium. Indeed, the system with $E=10$ is close to the strong field limit, in which the particle current is saturated to a constant value, and the equation of state for $E=10$ clearly deviates from the equilibrium one. This differ-
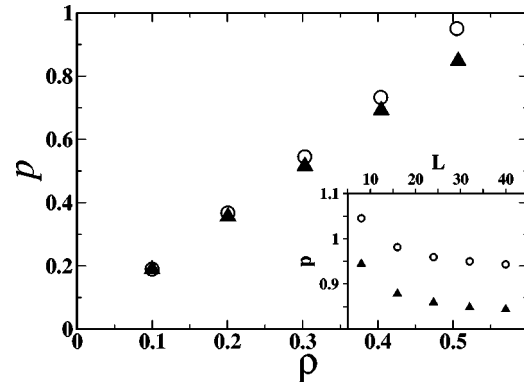


FIG. 1. Pressure as a function of the density average at the center of the system. The circular and triangular symbols correspond to the cases $E=0$ and $E=10$, respectively. Here, $M=L = 32$, $\Delta w = 0.4 \times 10^{-5}$, $w_m = 30$, and $t_0 = 16\,000$ (mcs). The averaged values for 100 samples are plotted. The statistical error bars are smaller than the symbols. The inset displays the $L$ dependence of the pressure with $N/L^2 = 0.5$ and $L/M = 1$. The pressure seems to converge to a definite value in the thermodynamic limit.

ence shows that the statistical distribution in the $y$ direction differs from the equilibrium one. Also, the pressure becomes an intensive variable in the thermodynamic limit, as seen in the inset of Fig. 1.

### CHEMICAL POTENTIAL

The chemical potential is measured by placing a particle reservoir in contact with the system in the direction transversal to the driving field. We first assume that the chemical potential of the reservoir, $\mu_R(T, \rho_R)$, is known. We also assume that there exists a chemical potential $\mu$ in this NESS that is a function of $T$, $\rho$, and $E$. From the definition of the chemical potential, we should have $\mu(T, \rho, E) = \mu_R(T, \rho_R)$. Then, using $\mu(T, 1-\rho, E) = \mu_R(T, 1-\rho_R)$, which holds due to the particle-hole symmetry, the equality $\mu(T, \rho=1/2, E) = \mu_R(T, \rho_R = 1/2)$ is derived. Thus, by measuring $\partial \mu(T, \rho, E)/\partial \rho$ for all values of $\rho$ without contacting a particle reservoir, we can determine the form of the function $\mu(T, \rho, E)$.

In order to measure $\partial \mu(T, \rho, E)/\partial \rho$ numerically, we add the one-body potential term $\sum_i \sigma_i \phi_i$ to the Hamiltonian $H(\sigma)$, where $\phi_i = \Delta\phi$ for $i_y \geq M/2+1$ and $\phi_i = 0$ for $i_y \leq M/2$. We then measure the density profile along the $y$ direction, in which there are two flat regions, $1 \leq i_y \leq M/2$ and $M/2+1 \leq i_y \leq M$. We denote the density in the region $1 \leq i_y \leq M/2$ as $\rho_1$ and the density in the region $M/2+1 \leq i_y \leq M$ as $\rho_2$. When $\Delta\phi$ is sufficiently small, the chemical potentials of the two regions are equal by the definition of the chemical potential. By taking into account the shift in the potential energy, this condition can be written as

$$\mu(T, \rho_1, E) = \mu(T, \rho_2, E) + \Delta\phi. \qquad (6)$$
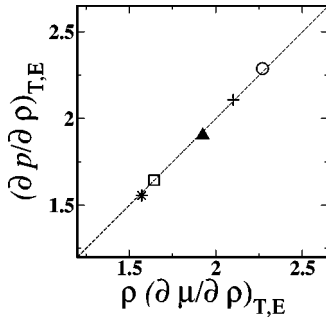
We thus obtain

FIG. 2. $\partial p(T,\rho,E)/\partial \rho$ vs $\rho \partial \mu(T,\rho,E)/\partial \rho$ for several values of $\rho$ and $E$. The triangle, square, star, plus, and circle correspond to $(\rho,E)=(0.5,10)$, $(0.4,10)$, $(0.3,10)$, $(0.5,3.0)$, and $(0.5,0.0)$, respectively. Here, $L=32$, and $M=32$ for $\partial p(T,\rho,E)/\partial \rho$ and $M=64$ for $\rho \partial \mu(T,\rho,E)/\partial \rho$. The statistical error bars are smaller than the symbols. The dotted line corresponds to the Maxwell relation.

$$\frac{\partial \mu(T,\rho,E)}{\partial \rho}\bigg|_{\rho=\bar{\rho}} = \lim_{\Delta\phi\to 0}\frac{\Delta\phi}{\Delta\rho}, \tag{7}$$

where $\Delta\rho=\rho_1-\rho_2$ and $\bar{\rho}=(\rho_1+\rho_2)/2$. Measuring $\Delta\rho$ and $\bar{\rho}$ for several values of $\Delta\phi$, we can evaluate the right-hand side of Eq. (7) [11].

### FREE ENERGY

We begin by conjecturing that the relation

$$\frac{\partial p(T,\rho,E)}{\partial \rho} = \rho \frac{\partial \mu(T,\rho,E)}{\partial \rho}, \tag{8}$$

which holds in equilibrium, holds also in our NESS. This is equivalent to the Maxwell relation because $p$ and $\mu$ are numerically confirmed to be intensive. Here, we estimate the value of $\partial p/\partial \rho$ (at $\rho=0.5$, for example) by calculating values of $p$ for several values of $\rho$ in a small interval around $\rho=0.5$ [11]. The results summarized in Fig. 2 suggest the validity of equality (8). If indeed this relation does hold, its implication is significant, because when we define the quantity $F(T,M,N,E)$ as

$$F(T,M,N,E)=N\mu\left(T,\frac{N}{ML},E\right)-MLp\left(T,\frac{N}{ML},E\right), \tag{9}$$

$p$ and $\mu$ become

$$p=-\frac{1}{L}\frac{\partial F(T,M,N,E)}{\partial M}, \tag{10}$$

$$\mu=\frac{\partial F(T,M,N,E)}{\partial N}. \tag{11}$$

That is, $F(T,M,N,E)$ can be regarded as the free energy extended to the present NESS. Using the single function $F(T,M,N,E)$, we can derive various thermodynamic relations, including the Clapeyron law, under nonequilibrium conditions.
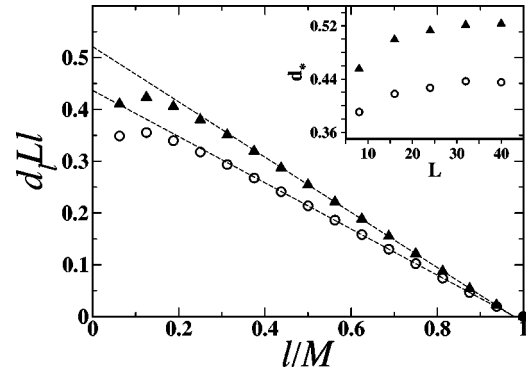


FIG. 3. $d_\ell L\ell$ as a function of $\ell/M$. Here, $L=M=32$. The statistical error bars are smaller than the symbols. The dotted line is obtained as the best fit line of the form $a\ell/M+b$ in the region $\ell/M\in[0.4,0.8]$ and $d_*$ is evaluated as the value of $b$. The inset displays the $L$ dependence of $d_*$ with the values $N/L^2=0.5$ and $L/M=1$ fixed. $d_*$ seems to converge to a definite value in the thermodynamic limit.

### FLUCTUATION RELATION

Consider the strip $\Omega_l=\{(i_x,i_y)|1\le i_x\le L, M/2-\ell/2-1\le i_y\le M/2+\ell/2\}$ and define the density variable $\rho_\ell=\Sigma_{i\in\Omega_l}\sigma_i/|\Omega_l|$, which is coarse grained over the strip $\Omega_l$. Let $\xi$ be the correlation length of density fluctuations in the $y$ direction. We define the free-energy density $f(\rho)$ for fixed $(T,E)$ by $F(T,M,N,E)=Mf(N/M)$ in the thermodynamic limit. It is then conjectured that the probability distribution of the density $\rho_\ell$ with $\xi\ll\ell\ll M$ (which is averaged over the $x$ direction) can be written as

$$P(\rho_\ell=\rho)\simeq\exp\{-\beta\ell[f(\rho)-f(\bar{\rho})]\}, \tag{12}$$

where $\bar{\rho}$ is the thermodynamic density. In the equilibrium case, such a form can be derived from a fundamental principle of statistical mechanics. Although there is no general proof of this form in the case of NESS, Eq. (12) seems plausible in the present case, because we have been able to define a free energy [13].

Recently, for some nonequilibrium lattice gases, the large deviation functionals of density fluctuations have been rigorously derived in nonlocal forms [5]. These nonlocal forms are related to long-range correlations that exist generically in NESS [12]. Here we shall not discuss this important issue further, and simply state our numerical finding that the scaling form (12) has been clearly observed, provided that one examines the density fluctuation in the strip $\Omega_\ell$ (note that the long-range density correlations transversal to the field do not seem to be observed [14]).

If Eq. (12) is valid (at least locally in the $y$ direction), the fluctuation relation

$$\beta\frac{\partial \mu}{\partial \rho}=\frac{1}{L\ell\langle(\rho-\bar{\rho})^2\rangle} \tag{13}$$

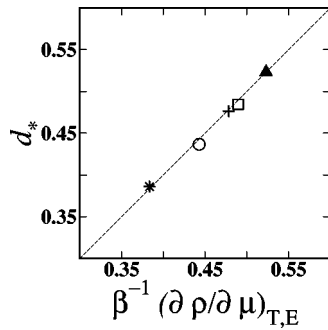can be derived. This relation is known to be valid for describing fluctuations about equilibrium states, but it is not

FIG. 4. $d_*$ vs $\beta^{-1}\partial\rho/\partial\mu$ for several values of $(\rho,E)$. The triangle, square, star, plus, and circle correspond to $(\rho,E)$ $=(0.5,10)$, $(0.4,10)$, $(0.3,10)$, $(0.5,3.0)$, and $(0.5,0.0)$, respectively. Here, $L=32$, and $M=32$ for $d_*$ and $M=64$ for $\beta^{-1}\partial\rho/\partial\mu$. The statistical error bars are smaller than the symbols. The dotted line corresponds to the fluctuation relation.

known whether it is valid in NESS. To study this point, we investigate Eq. (13) numerically.

We first note the asymptotic form

$$d_\ell \equiv \langle \rho_l^2 \rangle - \langle \rho_l \rangle^2 \simeq d_* \frac{1}{L\ell} \frac{M-\ell}{M} \quad (14)$$

for $\xi \ll \ell \ll M$ (see Fig. 3), where $d_*$ is defined. According to this, $L\ell\langle(\rho-\bar{\rho})^2\rangle$ in Eq. (13) should correspond to $d_*$. The values of $d_*$ and $\beta^{-1}\partial\rho/\partial\mu$ are plotted in Fig. 4. This result suggests the validity of Eq. (13). In addition, combining Eq.

(13) with Eq. (8), the relation we obtain between the compressibility and density fluctuations is the same as that existing in equilibrium.

We remark here that the asymptotic form (14) can be understood by considering the following simple situation. Consider $n$ random variables $x_i$ ($1\leqslant i\leqslant n$), with the conservation constraint $\Sigma_{i=1}^{n}x_i=0$. The statistical properties of $x_i$ are given by $E(x_i)=0$ and $E(x_ix_j)=\delta_{ij}$, where $E(x)$ represents the expected value of the random variable $x$. Let $X_k$ be the partial sum of $k$ elements randomly chosen from the set $\{x_i\}$. Then, the probability of $X_k$ with large $k$ and large $n-k$ is given by the Gaussian distribution with $E(X_k)=0$ and $E(X_k^2)=k(n-k)/n$ [15]. This supports the form of Eq. (14).

## DISCUSSION

We have presented relations obtained using numerical experiments on a driven lattice gas. We hope that the present study can be extended to a wider variety of systems. Also, finding a connection between the entropy, which is defined as $-(\partial F/\partial T)_{M,N,E}$ in our formulation, and the Shannon entropy would be important in future construction of a statistical mechanical theory of NESS [16].

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