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Nonequilibrium Steady States in Contact: Approximate Thermodynamic Structure and Zeroth Law for Driven Lattice Gases

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We explore driven lattice gases for the existence of an intensive thermodynamic variable which could determine "equilibration" between two nonequilibrium steady-state systems kept in weak contact. In simulations, we find that these systems satisfy surprisingly simple thermodynamic laws, such as the zeroth law and the fluctuation-response relation between the particle-number fluctuation and the corresponding susceptibility remarkably well. However, at higher densities, small but observable deviations from these laws occur due to nontrivial contact dynamics and the presence of long-range spatial correlations.

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Among the wide set of classes of nonequilibrium systems, an important and ubiquitous subclass is that which has a nonequilibrium steady state (NESS). Unlike in equilibrium, a system in a NESS has a steady current but its macroscopic properties, like in equilibrium, are still independent of time. In contrast to equilibrium systems, there is no well founded thermodynamic theory even for this conceptually simplest class of nonequilibrium systems. Intensive studies attempting to construct a suitable statistical mechanical framework where macroscopic properties and thermodynamic states may be characterized in a simple way have not yet converged to a universal picture [1–5].

At the heart of equilibrium thermodynamics is the zeroth law which is a consequence of equalization of intensive thermodynamic variables when two systems are in contact. For example, when two systems with the same temperature are allowed to exchange particles with the total number of particles conserved, the final equilibrium state is determined by equalization of the chemical potentials of the two, obtained by minimizing the total free energy. For NESSs, we ask the same: What happens if two NESSs are brought into contact?

Recently, there have been attempts to define an intensive thermodynamic variable for systems such as driven granular systems [6], static granular assemblies of blocked states formed by weak driving [7] and a class of exactly solvable models motivated by inelastic granular collisions [8]. More generally, there has been a prescription to define such a variable for systems in NESSs by invoking a hypothesis, called the asymptotic factorization property, which has been shown to be satisfied for a class of systems having short-range spatial correlations [9].

For driven diffusive systems like the paradigmatic stochastic lattice gases [10,11], which have long-range spatial correlations, the situation is less clear. Previously, motivated by equilibrium thermodynamics which has a rigorous basis in terms of the large-deviation principle (LDP) [12], a hypothesis of the existence of LDP has been put forward for these systems [1], but not yet rigorously established. By operationally defining a pressure and a chemical potential, a numerical study [13] indicates that a Maxwell relation is satisfied and there may indeed exist a large-deviation function analogous to the equilibrium free energy.

In equilibrium, the existence of an intensive variable hinges crucially on the local thermodynamic properties of a system, i.e., if the system is divided into subsystems large compared to the microscopic scales, the fluctuations in the individual subsystems are independent of each other as a consequence of the short-range spatial correlations in the system. In contrast, the driven systems have generic long-range spatial correlations [14]. In this situation, it is not obvious that the system could be divided into independent subsystems and intensive variables analogous to those in equilibrium could be defined.

In this Letter we explore by simulations the equilibration between two driven lattice gases upon contact. Interestingly, we find that, to a very good approximation, there is an intensive variable, like equilibrium chemical potential, which determines the final steady state while two such driven systems are allowed to exchange particles. Concomitantly, the zeroth law of thermodynamics is satisfied remarkably well. Moreover, a fluctuation-response relation between the fluctuations in particle-number and the corresponding susceptibility is also well satisfied. However, at higher densities, there are small but observable deviations from these simple thermodynamic laws due to nontrivial contact dynamics and the presence of long-range spatial correlations.

We consider two systems of volume V_1 and V_2, connected at a finite set of points $\tilde{V}_1$ and $\tilde{V}_2$ which are subsets of V_1 and V_2 respectively, with $\tilde{V}_1$, $\tilde{V}_2 \ll V_1$, V_2 (see Fig. 1). The two systems can interact and exchange particles with each other only at the contact. The energy H of the two systems combined is given by $H = K_1 \sum \eta(\mathbf{r_1})\eta(\mathbf{r'_1}) + K_2 \sum \eta(\mathbf{r_2})\eta(\mathbf{r'_2}) + \tilde{K} \sum \eta(\tilde{\mathbf{r}}_1)\eta(\tilde{\mathbf{r}}_2)$ where sums are over nearest-neighbor sites with $\mathbf{r_1}$, $\mathbf{r'_1} \in V_1$, $\tilde{\mathbf{r}}_1 \in \tilde{V}_1$ and $\mathbf{r_2}$, $\mathbf{r'_2} \in V_2$, $\tilde{\mathbf{r}}_2 \in \tilde{V}_2$. A site $\mathbf{r}$ can

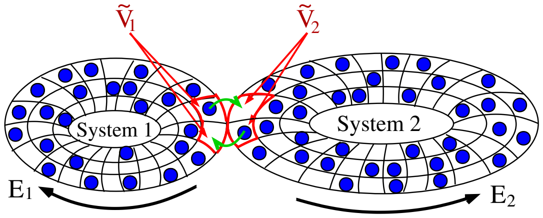

FIG. 1 (color online). A schematic diagram of two nonequilibrium steady states with contact region $\tilde{V}_1$ and $\tilde{V}_2$.

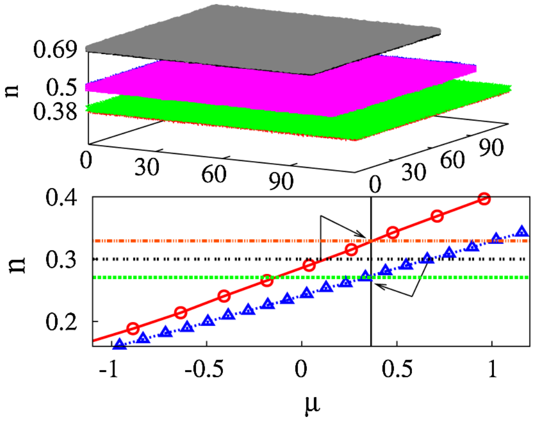

FIG. 2 (color online). Bottom panel: The plot of density n vs chemical potential μ for two 120×120 systems, NESS$_1$ with $K = 1$, $E = 2$ (circles) and NESS$_2$ with $K = E = 2$ (triangles) with $\tilde{K} = 0$. Arrows indicate how the density changes if NESS$_1$ and NESS$_2$ with the same initial density $n = 0.30$ (denoted by middle horizontal line) are brought into contact, reaching respective final densities $n \simeq 0.33$ (denoted by top horizontal line) and $n \simeq 0.27$ (denoted by bottom horizontal line) with equal chemical potential $\mu \simeq 0.36$. Top panel: Numerical experiments to test zeroth law ($\tilde{K} = 0$)—(1) NESS$_1$ ($K = 4$, $E = 6$, $L = 120$) with density n_1 (bottom red profile) equilibrated with NESS$_2$ ($K = E = 2$, $L = 110$) with density n_2 (middle blue profile), (2) NESS$_2$ with density n_2 (middle magenta profile) equilibrated with EQ$_1$ ($K = 1$, $E = 0$, $L = 100$) with density n_3 (top grey profile), and (3) NESS$_1$ with density n_1' (bottom green profile) equilibrated with EQ$_1$ with density n_3' (top black profile) where $n_1' \approx n_1$ and $n_3' \approx n_3$.

be occupied by at most one particle and the occupation variable $\eta(\mathbf{r})$ is 1 or 0 if the site is occupied or unoccupied, respectively. K_1, K_2 and $\tilde{K}$ are the interaction strengths among particles for system 1 and 2, and at the contact, respectively. In the simulations, we consider two-dimensional systems ($V = L \times L$) with periodic boundaries in both directions. We choose the jump rate $w(C'|C)$ from a configuration C to C' according to the local detailed balance condition [11]: the jump rate from a site $\mathbf{r}$ to its unoccupied nearest-neighbor $\mathbf{r}'$ obeys $w(C'|C) = w(C|C') \exp[-\Delta H + E(x' - x)]$, where $\Delta H = H(C') - H(C)$, E is the driving field along the x direction, and x and x' are x components of $\mathbf{r}$ and $\mathbf{r}'$ ($k_B T = 1$, k_B the Boltzmann constant, T temperature).

We choose $E = E_1$ when $\mathbf{r}$, $\mathbf{r}' \in V_1$, $E = E_2$ when $\mathbf{r}$, $\mathbf{r}' \in V_2$ and $E = 0$ otherwise. There is *no* driving field along the bonds connecting the two systems. We choose K_1, $K_2 > 0$ and E_1, E_2 so that systems are in the disordered (fluid) phase [10]. For $E_1 = E_2 = 0$, the combined system has the equilibrium Boltzmann distribution $\sim \exp[-H(C)]$. For $E_1, E_2 \neq 0$, there are currents in the steady states and the steady-state distribution is, in general, unknown. Driven bilayer systems were studied previously [15] where particles jump from one layer to the other at any site as opposed to the case here with possibility of particle transfer only at a small contact area.

We first report an *a priori* surprising observation suggesting an effective zeroth law for systems in NESS. When two systems are brought into contact, after relaxation involving exchange of particles, in the final "equilibrated" steady state there is no net current across the contact region. This property allows an operational definition of a chemical potential of a NESS as follows. A driven system is brought into contact with an equilibrium system EQ whose chemical potential μ is known as a function of density. In the final steady state, the chemical potential μ of EQ is assigned to the driven system. We choose a system of noninteracting hard-core particles as EQ with density being n_0 and $\mu = -(\partial s/\partial n_0) = \ln[n_0/(1 - n_0)]$ with $s = -[n_0 \ln n_0 + (1 - n_0) \ln(1 - n_0)]$ the equilibrium entropy per lattice site. By varying n_0 of EQ in contact with a NESS in consideration, one can get the density versus chemical potential curve for the NESS as shown in Fig. 2 (bottom panel). The surprising observation is that, if two NESSs, NESS$_1$ and NESS$_2$ (chosen such that they have operationally the same μ but different densities), are brought together, the respective densities do not change upon contact. Moreover, if we bring together two NESSs with the same density but different μ, particles will flow from the higher to lower chemical potential till the respective densities correspond to the same μ as indicated with arrows in Fig. 2 (bottom panel).

Thus, if two systems are separately equilibrated with a common system with a fixed density, they will also be equilibrated amongst themselves. Consider, e.g., two systems NESS$_1$ and NESS$_2$ kept in contact and having two equilibrated density profiles, with density n_1 and density n_2, respectively. Then, a third system EQ$_1$ is separately brought into contact with NESS$_2$ and the density of EQ$_1$ is tuned to n_3 such that NESS$_2$ keeps its density n_2 unchanged in the equilibrated state. Now, if NESS$_1$ with density n_1 and EQ$_1$ with density n_3 are brought into contact, the two density profiles remain almost unchanged, confirming the zeroth law (see Fig. 2, top panel and the explanations in the caption).

These systems are indeed far away from equilibrium since the numerical values of the currents in NESS$_1$ and NESS$_2$ in the bottom panel of Fig. 2 are approximately $2/3$ and $1/3$ of the respective maximum currents. Likewise, in the top panel, NESS$_2$ with density ≈ 0.5 has a homogeneous disordered state in contrast to the corresponding equilibrium system, with $K = 2$, $E = 0$ and the same density, which has a symmetry-broken phase with different sublattice densities [10].

The chemical potential of a system may also be measured by keeping it in contact with any other equilibrium system, not necessarily a noninteracting hard-core one. In Fig. 3, we have plotted densities versus chemical potentials for a system separately in contact with systems with different contact area as well as nonzero interaction strength $\tilde{K}$, the result being in good agreement with the zeroth law.

The existence of a zeroth law would be a consequence of a putative large-deviation principle (LDP) [12]. To elucidate it briefly, let us consider two systems which can exchange particles such that $N_1 + N_2 = N = \text{const}$, N_1, N_2 the number of particles in systems 1 and 2, respectively. Assuming that the LDP holds, the probability $P(N_1, N_2)$ of a large deviation in N_1, N_2 is given by $P(N_1, N_2) \sim [e^{V_1 s_1(n_1)} e^{V_2 s_2(n_2)}] e^{-S(N)}$ in the limit of N_1, N_2, V_1, $V_2 \gg 1$, where $n_1 = N_1/V_1$ and $n_2 = N_2/V_2$ being finite and $\exp[-S(N)]$ the normalization constant ("$\sim$" implying equality in terms of logarithm). The functions $s_1(n_1)$, $s_2(n_2)$ are called the large-deviation functions (LDF). In writing so, the correlation between systems has been neglected as a boundary-effect in the limit of large volume. This assumption of a product measure of $P(N_1, N_2)$ essentially implies that the LDFs $s_1(n_1)$ and $s_2(n_2)$ are local function of the respective densities. The macroscopic state, under the constraint $N_1 + N_2 = \text{const}$, is determined by maximizing $\ln P(N_1, N_2)$ where the chemical potentials $\mu_1 = -\partial s_1/\partial n_1$ and $\mu_2 = -\partial s_2/\partial n_2$ being equal in the final steady-state. Clearly the consequence of the LDP is a zeroth law as presented in Fig. 2. Another interesting consequence of a putative LDP would be a relation between the susceptibility and the fluctuation in particle-number of the system 1 in a NESS when it is in contact with the system 2 being a large reservoir characterized by a chemical potential μ. Then, one gets the following fluctuation-response relation as in equilibrium,

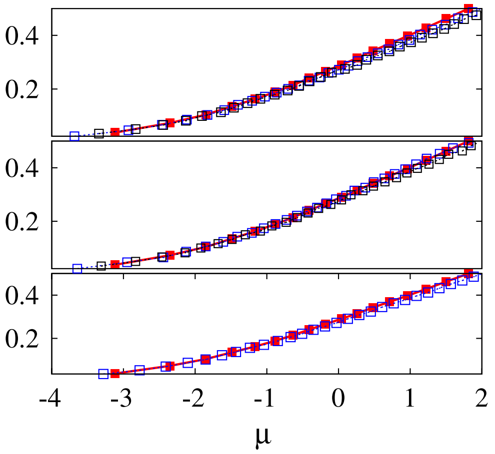

FIG. 3 (color online). Density n vs chemical potential μ is plotted for a 120×120 NESS$_1$ ($K = 1$, $E = 2$) for the following cases. Bottom panel: NESS$_1$ separately in contact with 120×120 systems with EQ$_1$ ($K = E = 0$, red) and EQ$_2$ ($K = 1$, $E = 0$, blue). Middle panel: NESS$_1$ separately in contact with EQ$_1$ (blue) and EQ$_2$ (black) with 4×1 contact area. Top panel: NESS$_1$ separately in contact with EQ$_1$ (blue) and EQ$_2$ (black) for nonzero interaction strength $\tilde{K} = 1$. In middle and top panel, n vs μ plot is compared with that obtained for NESS$_1$ in contact with EQ$_1$ with 2×2 contact area.

$$\chi \equiv \frac{\partial \langle N_1 \rangle}{\partial \mu} = (\langle N_1^2 \rangle - \langle N_1 \rangle^2) \equiv \sigma_{N_1}^2. \qquad (1)$$

We first proceed to test this relation for a NESS in contact with an equilibrium reservoir with density n_0, consisting of noninteracting hard-core particles with $\mu = -(\partial s/\partial n_0) = \ln[n_0/(1 - n_0)]$. For better numerical accuracy, we check the integrated version of Eq. (1) by defining the integrated susceptibility $I_\chi(\mu) \equiv \int_{\mu_0}^{\mu} (\partial \langle N_1 \rangle / \partial \mu) d\mu = \langle N_1(\mu) \rangle - \langle N_1(\mu_0) \rangle$ and the integrated fluctuation $I_\sigma(\mu) \equiv \int_{\mu_0}^{\mu} (\sigma_{N_1}^2) d\mu$.

We take a 20×20 nonequilibrium system NESS$_1$ with $K = 1$, $E = 2$ and keep it in contact with a 100×100 equilibrium reservoir of noninteracting hard-core particles ($K = E = 0$), called RES$_1$. Then we vary the chemical potential μ (or, equivalently, the density n_0) of RES$_1$ in small steps from an initial value $\mu_0 = -3.5$ and calculate $\sigma_{N_1}^2$ for each value of μ. We repeat this procedure by keeping NESS$_1$ separately in contact with various other reservoirs of size 100×100 whose chemical potentials can be measured by keeping these reservoirs in contact with the RES$_1$. In Fig. 4, we plot $I_\chi(\mu)$ and $I_\sigma(\mu)$ as a function of μ. Provided that the Eq. (1) is valid, all the curves should fall on each other. Up to chemical potential $\mu \simeq 1$, we observe a quite good collapse within the numerical accuracy. We also consider two different systems, NESS$_1$ with $K = 1$, $E = 2$ and NESS$_2$ with $K = E = 2$, separately in contact with RES$_1$. In the inset of Fig. 4, we plot $I_\chi(\mu)$ and $I_\sigma(\mu)$ which are in good agreement with the fluctuation relation in Eq. (1).

At higher chemical potentials, there are observable deviations from this simple thermodynamic behavior. In Fig. 4, the I_χ vs μ and I_σ vs μ curves do not fall on each other for $\mu \gtrsim 1$. Correspondingly, in this density regime, the zeroth law does not hold strictly as seen in Fig. 3. However, these violations are not simply due to a finite-size effect and persist for much larger system sizes. To investigate the possible reasons for the violations, we also study the behavior of spatial density correlation functions for various densities. Unlike equilibrium systems, the nonequilibrium systems, due to the presence of a driving field, are expected to have generic long-range spatial correlations [10,14,16,17], arising because the structure factor

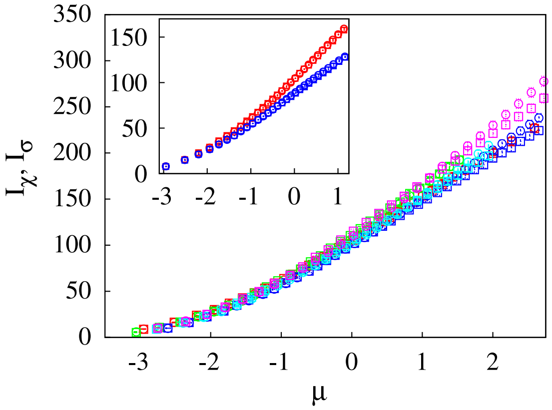

FIG. 4 (color online). Integrated susceptibilities I_χ (squares) and fluctuations I_σ (circles) vs chemical potential μ are plotted for a 20×20 NESS_1 with $K = 1$, $E = 2$, separately in contact with five different 100×100 reservoirs: (1) $K = E = 0$ (red), (2) $K = 1$, $E = 2$ (green), (3) $K = 1$, $E = 4$ (blue), (4) $K = 2$, $E = 4$ (sky-blue), (5) $K = 2$, $E = 6$ (magenta). Inset: Same quantities are plotted for two different 20×20 systems, NESS_1 with $K = 1$, $E = 2$ (blue) and NESS_2 $K = E = 2$ (red), in contact with a reservoir ($K = E = 0$, $L = 100$).

$S(q_x, q_y)$, i.e., the Fourier transform of the spatial density correlation function, becomes singular when q_x, $q_y \to 0$ with $R = [\lim_{q_y \to 0} S(0, q_y)]/[\lim_{q_x \to 0} S(q_x, 0)] \neq 1$. This gives rise to the long-range spatial correlations decaying as A/r^d with distance r in d dimension with the amplitude $A \propto (R - 1)$ [10]. In Fig. 5, we have plotted the ratio R versus density n and the structure factors $S(q_x, 0)$ and $S(0, q_y)$ for two different densities in inset of Fig. 5 for a NESS with $K = 1$, $E = 2$, $L = 120$. The ratio R deviates from 1 more strongly with increasing density, indicating an increase of long-range correlations which manifest themselves through the nonlocal effect of the contact. In Figs. 3 and 4, collapse of various n vs μ and I_σ vs μ (or I_χ vs μ) curves for different contact dynamics are not very good for $\mu \gtrsim 1$. Clearly, the effect of the contact is felt throughout the systems and this nontrivially changes the corresponding thermodynamic properties. Therefore, the breakdown of an exact equilibriumlike structure or, in other words the breakdown of the product-measure assumption in the LDP, indicates the important role of the contact dynamics [9] and the long-range correlations in a driven system.

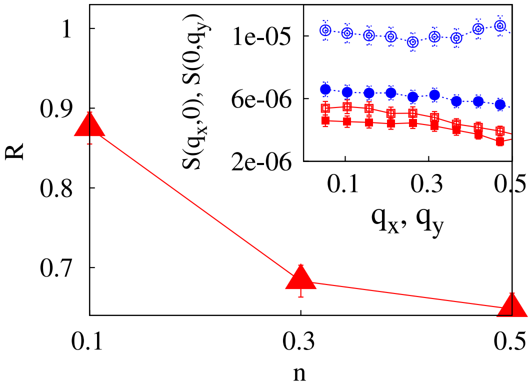

FIG. 5 (color online). The ratio $R = [\lim_{q_y \to 0} S(0, q_y)]/[\lim_{q_x \to 0} S(q_x, 0)]$ vs density n is plotted for a NESS with $K = 1$, $E = 2$, $L = 120$. Inset: The structure factors $S(q_x, 0)$ (open points) and $S(0, q_y)$ (filled points) vs q_x and q_y respectively are plotted for densities $n = 0.1$ (red) and $n = 0.5$ (blue).

In summary, our numerical study of coupled driven lattice gases has revealed a surprisingly simple thermodynamic structure with an effective zeroth law like behavior concerning exchange of particles and the corresponding fluctuation-response relation. This thermodynamic structure is not exact since there are small but observable deviations at higher densities. Their physical origin is rooted in the nontrivial contact dynamics and the presence of long-range spatial correlations which invalidate the asymptotic factorization property. As an open question, it would be interesting to see whether systems with more than one conserved quantity (e.g., models with two species) exhibit a similar behavior. Finally our study prompts the question whether such an approximate thermodynamic structure is typical just for driven lattice gases or generically occurs in other coupled NESSs with long-range correlations as well.

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[1] G. L. Eyink *et al.*, J. Stat. Phys. **83**, 385 (1996).
[2] Y. Oono and M. Paniconi, Prog. Theor. Phys. Suppl. **130**, 29 (1998).
[3] L. Bertini *et al.*, Phys. Rev. Lett. **87**, 040601 (2001).
[4] T. Bodineau and B. Derrida, Phys. Rev. Lett. **92**, 180601 (2004).
[5] S. Sasa and H. Tasaki, J. Stat. Phys. **125**, 125 (2006).
[6] H-Q Wang and N. Menon, Phys. Rev. Lett. **100**, 158001 (2008).
[7] S. Henkes, C. S. O'Hern, and B. Chakraborty, Phys. Rev. Lett. **99**, 038002 (2007).
[8] Y. Shokef, G. Shulkind, and D. Levine, Phys. Rev. E **76**, 030101(R) (2007).
[9] E. Bertin, O. Dauchot, and M. Droz, Phys. Rev. Lett. **96**, 120601 (2006); E. Bertin *et al.*, Phys. Rev. E **75**, 031120 (2007).
[10] B. Schmittmann and R. K. P. Zia, Phys. Rep. **301**, 45 (1998); R. K. P. Zia, J. Stat. Phys. **138**, 20 (2010).
[11] S. Katz *et al.*, J. Stat. Phys. **34**, 497 (1984).
[12] H. Touchette, Phys. Rep. **478**, 1 (2009).
[13] K. Hayashi and S. I. Sasa, Phys. Rev. E **68**, 035104 (2003).
[14] J. R. Dorfman *et al.*, Annu. Rev. Phys. Chem. **45**, 213 (1994).
[15] A. Achahbar and J. Marro, J. Stat. Phys. **78**, 1493 (1995); C. C. Hill, R. K. P. Zia, and B. Schmittmann, Phys. Rev. Lett. **77**, 514 (1996).
[16] P. L. Garrido *et al.*, Phys. Rev. A **42**, 1954 (1990).
[17] G. Grinstein, D. H. Lee, and S. Sachdev, Phys. Rev. Lett. **64**, 1927 (1990).