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Failure of steady-state thermodynamics in nonuniform driven lattice gases

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To be useful, steady-state thermodynamics (SST) must be self-consistent and have predictive value. Consistency of SST was recently verified for driven lattice gases under global weak exchange. Here I verify consistency of SST under local (pointwise) exchange, but only in the limit of a vanishing exchange rate; for a finite exchange rate the coexisting systems have different chemical potentials. I consider the lattice gas with nearest-neighbor exclusion on the square lattice, with nearest-neighbor hopping, and with hopping to both nearest and next-nearest neighbors. I show that SST does not predict the coexisting densities under a nonuniform drive or in the presence of a nonuniform density provoked by a hard wall or nonuniform transition rates. The steady-state chemical potential profile is, moreover, nonuniform at coexistence, contrary to the basic principles of thermodynamics. Finally, I discuss examples of a pair of systems possessing *identical steady states* but which *do not coexist* when placed in contact. The results of these studies confirm the validity of SST for coexistence between spatially uniform systems but cast serious doubt on its consistency and predictive value in systems with a finite rate of particle exchange between coexisting regions exhibiting a nonuniform particle density.

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I. INTRODUCTION

A central issue in nonequilibrium physics is whether thermodynamics can be extended to systems far from equilibrium [1–6]. Such a theory would be a macroscopic description employing a small number of variables, capable of predicting the final state of a system following removal of some constraint [7]. Although the set of variables needed to describe a nonequilibrium system would be somewhat larger than required for equilibrium, it should not involve microscopic details. Near-equilibrium thermodynamics, for example, includes the fluxes of mass, energy, and other conserved quantities as relevant variables [8,9].

In this context, a natural first step is to develop a thermodynamics of nonequilibrium steady states (NESS) and to analyze the simplest possible examples exhibiting such states, for example, driven stochastic lattice gases [10–13] or the asymmetric exclusion process [14]. A detailed theory of hydrodynamics and fluctuations in driven diffusive systems was developed by Eyink *et al.* [15]. Sasa and Tasaki [16], extending the ideas of Ref. [1], proposed a general scheme of steady-state thermodynamics (SST), including definitions of the chemical potential and pressure in NESS, and developed a theoretical analysis of the driven lattice gas; numerical implementations in driven systems are discussed in Refs. [3,17]. More recently, Chatterjee *et al.* [18] established that in driven systems with particle number conservation and short-ranged correlations, fluctuations in the particle number n_s of a subsystem are determined by the functional relation between the variance and the mean of n_s. They argued that this guarantees the existence of a chemical potential.

A central notion in SST is that of *coexistence*. Consider two systems, each in a steady state, and weakly coupled to one another, so they may exchange particles and/or energy. We say that the systems coexist when the net flux of the quantity or quantities they may exchange is zero. In equilibrium, coexistence in this sense corresponds to chemical and/or thermal equilibrium, marked by equality of μ/T and T, respectively (μ denotes chemical potential and T temperature). To construct a SST, we need to define intensive parameters for NESS, such that the value of the parameter associated with particle exchange (a dimensionless chemical potential, μ/T) is the same when two systems coexist with respect to such exchange and, similarly, an effective temperature, T, if the systems coexist with respect to energy exchange. The definition of intensive parameters for nonequilibrium systems (such as the zero-range process) possessing an asymptotic factorization property has been discussed in considerable detail by Bertin *et al.* [4]. Direct numerical tests of the consistency of SST (that is, of the zeroth law) under particle exchange were performed by Pradhan *et al.* [17] in the context of the driven lattice gas with nearest-neighbor interactions (i.e., the Katz-Lebowitz-Spohn (KLS) model [10]). These authors noted small but significant violations of the zeroth law. The results of Ref. [19] suggest that such inconsistencies arise because (1) one needs to define an effective temperature as well as an effective chemical potential in the KLS model, (2) one needs to use rates of the Sasa-Tasaki type for exchange between systems [20], and (3) one needs to study the limit of vanishing rate of particle exchange between the systems under analysis. When these conditions are satisfied, the zeroth law holds [19].

The results of Ref. [19] are restricted to spatially uniform systems; here I take the first steps toward verifying SST in nonuniform systems. A particularly simple testing ground for SST is athermal lattice gases, in which the intensive variable of interest is $\mu^* \equiv \mu/k_BT$, which I shall call the chemical potential in what follows. In equilibrium, $\mu^* = \mu^*(\rho)$, with ρ the particle density. In a system subject to a nonequilibrium drive D, one might hope to define a function $\mu^*(\rho,D)$ using coexistence between the driven system and an equilibrium

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reservoir of known chemical potential. A recent study [19] confirmed that for driven athermal lattice gases with nearest-neighbor (NN) exclusion, one may indeed define a function $\mu^*(\rho,D)$ in this manner: Under global weak exchange, the coexisting densities in a pair of systems with different values of D are given by the condition of equal chemical potentials, i.e., $\mu^*(\rho,D) = \mu^*(\rho',D')$, where μ^* describes an *isolated* system. *Global* exchange means that any particle in one system may jump to any site in the other (provided, of course, that the target site and its nearest neighbors are all vacant). *Weak* exchange corresponds to the limit of the exchange rate p_r tending to zero. Important consequences of weak exchange are (1) the systems in contact are statistically independent and (2) particle exchange does not provoke spatial variations within these systems.

Although the consistency observed in this rather restricted and artificial situation is encouraging, for SST to be relevant to laboratory conditions, it must be tested in more realistic settings. In particular, the global exchange scheme mentioned above would seem to be far from experimental reality. Here I begin by studying the opposite case, in which exchange is allowed only between a single pair of sites, mimicking a situation in which two systems have a very small area of contact. I then turn to the NNE lattice gas subject to a *nonuniform* drive (corresponding to systems in contact along a line) and to situations in which a nonuniform particle density arises due to a hard wall or to reduced hopping rates along a line parallel to the drive. In these cases the predictions of SST are violated dramatically. Finally I consider coexistence between systems with all transition rates having the same ratios, differing only by an overall multiplicative factor. Since stationary properties are invariant under rescaling of time, these systems possess the same steady state. I find, nevertheless, that when the systems make contact along a line they do not coexist: particles migrate from one system to the other.

I consider the lattice gas with NN exclusion on the square lattice, with two kinds of dynamics: (i) nearest-neighbor hopping (NNE dynamics) and (ii) hopping to both nearest and next-nearest neighbors (NNE2 dynamics). Under a drive D that favors hopping along one direction, the system attains a NESS. When the drive is only applied to half the system we have (in the steady state) coexistence between a pair of subsystems, one in equilibrium and the other far from equilibrium, able to exchange particles along the interfaces separating them. Let the bulk particle densities in the driven and undriven regions be ρ_D and ρ_0, respectively. A key question is whether the condition $\mu^*(\rho_D,D) = \mu^*(\rho_0,0)$ allows us to predict the coexisting densities, in other words, whether SST has predictive value for this system.

The balance of this paper is organized as follows. In Sec. II I define the models and review the relevant properties of the isolated systems. Section III presents simulation results for exchange between single sites, followed, in Sec. IV, by those for a system under a nonuniform drive, and in Sec. V, for those involving walls or barriers. In Sec. VI I discuss the results for contact between systems with transition rates differing only by an overall factor; I close in Sec. VII with a discussion of the implications of the results for steady-state thermodynamics.

II. LATTICE GASES WITH NEAREST-NEIGHBOR EXCLUSION

The lattice gas with NN exclusion is a particle model with a pairwise interaction that is infinite for distances of zero and unity (in units of the lattice constant) and zero otherwise. Thus each particle excludes others from occupying its own site or any of its first neighbors. Since there is no characteristic energy scale, the relation between the density and the chemical potential $\mu^* = \mu/k_BT$ (and, similarly, between p/k_BT and ρ, where p is pressure) is independent of temperature. Such models are termed *athermal*. The model has been studied extensively as a discrete-space version of the hard-sphere fluid [21–24] and is known to exhibit a continuous (Isinglike) phase transition to sublattice ordering at a density of $\rho_c \simeq 0.36774$ [25].

We define a stochastic, particle-conserving dynamics for the lattice gas with NN exclusion via particle hopping. In the simplest case [13], particles are allowed to hop only to nearest-neighbor sites (the NNE model). In equilibrium (drive $D = 0$), detailed balance implies that $P(\mathbf{x}) = P(-\mathbf{x})$, where $P(\mathbf{x})$ denotes the probability of attempting a particle displacement $\mathbf{x}$. In the presence of a drive, the displacement probabilities on the square lattice are

$$P(\pm\mathbf{i}) = \frac{1 \pm D}{4}, \quad w(\pm\mathbf{j}) = \frac{1}{4}, \tag{1}$$

which reduce to the symmetric case for $D = 0$. Evidently, $D > 0$ favors displacements along the $+x$ axis. Given periodic boundaries along this direction, $D \neq 0$ represents a nonequilibrium situation, corresponding to a force that cannot be written as the gradient of a single-valued potential function. In the continuous-time stochastic evolution, each particle is equally likely to be the next to attempt to hop; the hopping direction is chosen according to Eq. (2). Any particle displacement satisfying the exclusion condition is accepted.

A defect of the hopping dynamics defined above is that it is nonergodic, independent of the drive [19]. This is remedied by allowing displacements to second- as well as first-neighbor sites. For this dynamics, which we denote as NNE2, the displacement probabilities are

$$P(\sigma\mathbf{i} + \eta\mathbf{j}) = \frac{1 + \sigma D}{8}, \tag{2}$$

for $\sigma \in \{-1,0,1\}$ and, similarly for η, excluding $\sigma = \eta = 0$. The enhanced set of possible displacements eliminates configurations inaccessible under NN hopping only. The phase diagram of the driven NNE2 model was studied some years ago by Szolnoki and Szabo [26], who showed that there is a line of Ising-like phase transitions in the ρ-D plane, with $\rho_c \simeq 0.35$ for $D = 1$.

In the lattice gas with NN exclusion, a site is *open* if it and all its NNs are vacant. (Particles can be inserted only at open sites.) In Ref. [19] it is shown that the chemical potential is given by

$$\mu^*(\rho,D) = \ln(\rho/\rho_{\mathrm{op}}), \tag{3}$$

where ρ_{op} is the average density of open sites over configurations with $n = \rho L^d$ particles. The above relation follows from coexistence with a particle reservoir and holds independently of the value of D and of the nature of the dynamics (NNE

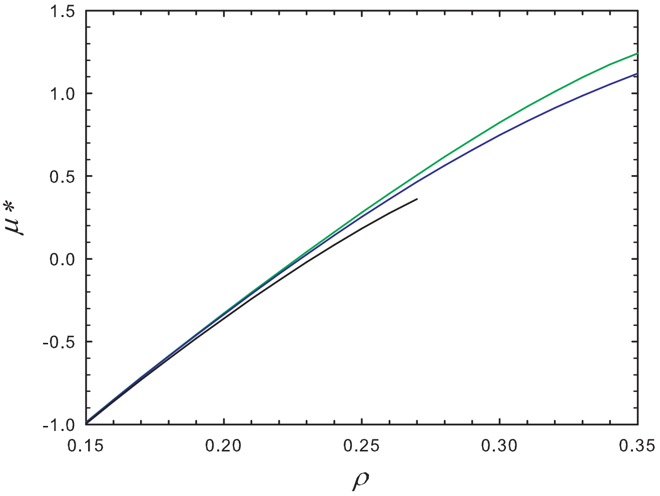

FIG. 1. (Color online) Chemical potential μ^* versus particle density ρ in the lattice gas with NN exclusion for (upper to lower) equilibrium, maximum drive ($D = 1$) under nearest- and next-nearest neighbor hopping (NNE2 dynamics), and maximum drive under nearest-neighbor hopping (NNE dynamics). Data are simulation results for the square lattice, system size $L = 80$. Uncertainties are smaller than the line width.

or NNE2). Our definition of μ^* is equivalent to the general definition proposed by Sasa and Tasaki [16]. It is also consistent with the zeroth law, as verified in Ref. [19].

The dependence of μ^* on the drive arises because, for a given particle density ρ, the density of open sites depends on D. The chemical potential is plotted versus particle density ρ in Fig. 1 for equilibrium and maximum drive ($D = 1$) under NNE and NNE2 dynamics. Evidently the drive causes a reduction in μ^*; the reduction is greater in the NNE case. (Note that the data are limited to densities smaller than the critical densities of the respective models.)

Studies reported in Ref. [19] show that if a pair of lattice gases, A and B, driven or not, are allowed to exchange particles, then in the weak-exchange limit the coexisting particle densities ρ_A and ρ_B are predicted by the condition $\mu^*(\rho_A, D_A) = \mu^*(\rho_B, D_B)$. This relation holds for both NNE and NNE2 dynamics. It is important to emphasize that this relation was verified in a highly idealized situation: The contact between systems is global, in the sense that any site in A can exchange a particle with any site in B. If one or both of the systems is driven, the chemical potentials of the isolated systems are useful in predicting the coexisting densities only in the limit that the exchange rate p_r tends to zero. (For finite p_r the chemical potentials of the coexisting systems are equal but differ from the values found for the systems in isolation.) In Ref. [19] global coupling is used to avoid any possible complication arising from inhomogeneities, such as localized exchange [17]. The weak-exchange limit is necessary because the strength of the nonequilibrium perturbation varies with p_r.

III. POINTWISE EXCHANGE

I study pointwise exchange between a driven and a nondriven system, implemented as follows. In each system (a lattice of $L \times L$ sites, with periodic boundaries), a fixed *exchange site* $\mathbf{x}_e$ is chosen. A fraction p_r of all attempted transitions are exchange attempts; exchange occurs when the exchange site of one system is occupied and the other vacant. The remaining transitions are particle displacements within each system, as described above. I consider the stationary behavior of the coupled systems. In the limit $p_r \to 0$, we expect the driven and nondriven systems to coexist, with equal values of μ^*, since this is the condition for zero particle flux, when the two systems can be treated as statistically independent [19]. (In this limit, each system has ample time to reestablish a translationally invariant state, uncorrelated to the other system, prior to the next exchange event.) For nonzero values of p_r the situation is more complicated, because of spatial nonuniformities and correlations between the two systems.

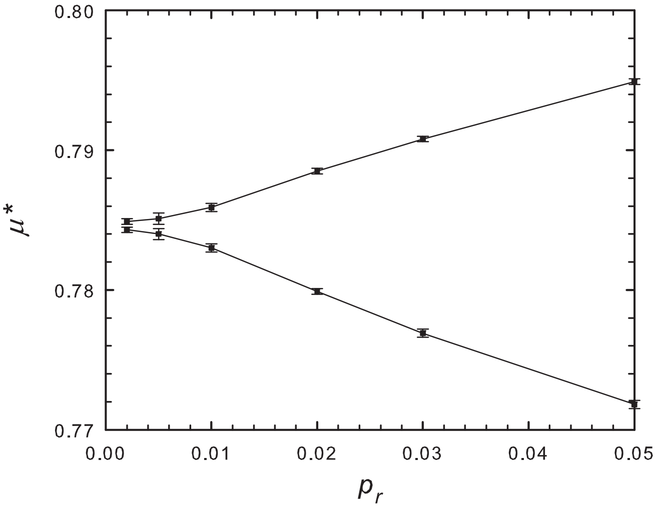

FIG. 2. Chemical potential μ^* versus exchange rate p_r under pointwise exchange (upper: driven system; lower: nondriven system) in the lattice gas with NNE2 dynamics. System size $L = 20$, mean density 0.3.

Numerical investigation reveals that the values of μ^* in the driven and nondriven system approach a common limiting value (that of coexistence) *only* as $p_r \to 0$; the stationary chemical potentials clearly differ for nonzero exchange rates, as shown in Fig. 2, for NNE2 dynamics. (The particle density in the driven system is consistently greater than that of the nondriven system.) In this study, for a global particle density of 0.3, the chemical potentials, extrapolated to $p_r = 0$, are 0.7847(2) and 0.7846(2) in the driven and nondriven systems, respectively. This result is in contrast with that obtained under *global* exchange [19], in which the chemical potentials are equal, albeit dependent on p_r; it suggests that the difference in μ^* values is associated with spatial nonuniformities, which are favored (disfavored) by pointwise (global) exchange. This is verified in Fig. 3, which shows the mean stationary particle density as a function of distance from the exchange site. (Since the profiles along and perpendicular to the drive are essentially identical, the average of the two profiles is shown in each case.) For finite p_r there are clear oscillations in the density profile; the latter decrease in amplitude as we reduce p_r. (The simulation times in studies of pointwise exchange are 2×10^9 time units, with the first half discarded to allow time for the

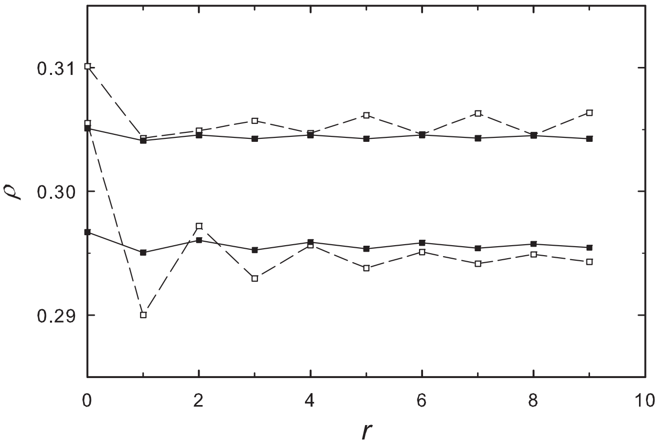

FIG. 3. Stationary particle density versus distance r from exchange site under pointwise exchange (upper: driven system; lower: nondriven system) in the lattice gas with NNE2 dynamics. Open symbols: $p_r = 0.05$; filled symbols: $p_r = 0.005$. Parameters as in Fig. 2.

system to reach the steady state; a time unit corresponds to one attempted move per particle. Although one would like to study smaller values of p_r and larger system sizes, this would entail significantly longer simulation times.)

Summarizing the results for coexistence under pointwise exchange, I verify that, as anticipated, stationary properties are correctly predicted by SST for a vanishing exchange rate. For finite p_r, however, equating chemical potentials of the driven and nondriven systems does not predict the coexisting densities; the chemical potentials of the coexisting systems are unequal. The discrepancy is associated with a nonuniform particle density. In the following sections I study intrinsically inhomogeneous systems.

IV. EXCHANGE ALONG AN EDGE

In this section I study a lattice of $L \times L$ sites divided into two parts by applying a nonzero drive in half of the system, that is, for sites (i,j) with $\frac{L}{2} + 1 \leqslant j \leqslant L$. Thus the boundaries between the driven and undriven regions (between $j = \frac{L}{2}$ and $\frac{L}{2} + 1$ and between $j = L$ and $j = 1$) are parallel to the drive. I report simulation results for the stationary density and chemical potential profiles [$\rho(j)$ and $\mu^*(j)$, respectively, the latter obtained via Eq. (3), with the j-dependent values of ρ and ρ_{op}]. If SST functions correctly, the coexisting bulk densities ρ_0 and ρ_D should be given by the equal chemical potential condition (implying $\rho_D > \rho_0$), and the chemical potential profile should be flat, $\mu^*(j) = \mu^*(\rho_0,0) = \mu^*(\rho_D,D)$.

A. NNE dynamics

I study the NNE lattice gas on square lattices of $L \times L$ sites (with periodic boundaries), with L ranging from 200 to 800. Initially, particles are distributed uniformly over the lattice by inserting particles at randomly chosen open sites. For the densities and system sizes considered here, the system attains a stationary state well before 5×10^6 time units, the time allowed for relaxation; averages are calculated over a period of 5×10^6–10^7 time units, following relaxation.

The stationary properties of the half-driven system are hardly what one would expect based on SST. Typical density and chemical potential profiles are shown in Fig. 4. The density is higher in the undriven region, contrary to the prediction obtained equating the chemical potentials of driven and undriven systems. The chemical potential profile is clearly nonuniform; more so, in fact, than if the particle density were uniform at the global density. Particles have migrated to increase severalfold the difference in chemical potential between the two regions, rather than diminish it. Varying the global density, the bulk densities observed in simulation consistently violate the expected tendency, that is, $\rho_D < \rho_0$; the difference grows with global density, as shown in Fig. 5.

The density and chemical potential profiles of Fig. 4 show well-defined bulk regions, justifying the interpretation of coexisting phases. The bulk density and chemical potential values, (ρ_0,μ_0^*) and (ρ_D,μ_D^*), fall on the corresponding curves, $\mu^*(\rho,D=0)$ and $\mu^*(\rho,D=1)$, characterizing the isolated systems. In other words, the driven and undriven regions retain their respective bulk properties in the presence of a nonuniform drive. I note that the chemical potential profile within the nondriven region is essentially flat, despite significant variations in density, as one would expect in an equilibrium system such as a fluid confined between repulsive walls. In the driven region, by contrast, the chemical potential profile varies over a substantial region ($\sim$10–20 lattice spacings) near the boundaries. In this region the excess chemical potential is well approximated by an exponential, $\Delta\mu^* \equiv \mu^*(x) - \mu_D^* \sim e^{-x/\lambda}$, where x denotes the distance from the boundary. The "healing length" λ grows with density; for a global density of 0.25, I find $\lambda \simeq 5.5$. The density profiles follow a similar pattern: the excess density, relative to the bulk values in the driven and nondriven regions, is again well approximated by an exponential, $\Delta\rho \sim e^{-x/\lambda}$, with $\lambda = 2.8(1)$ and $5.0(2)$ for overall densities 0.2 and 0.25, respectively, in the nondriven region and $\lambda = 2.55(2)$ and $6.30(2)$ for the same densities in the driven region. The amplitude of the excess density is considerably larger in the driven region (by a factor of $\sim$50 for $\rho = 0.25$).

Particles migrate to the undriven region, parallel to the chemical potential gradient (i.e., *contrary* to Fick's law), for all system sizes examined, as well as for a smaller drive ($D = 0.5$). Migration to regions of zero or weaker drive was noted (for low densities) in Ref. [27], in which the NNE model is subject to a drive which varies linearly with position j in the direction perpendicular to the drive. In Ref. [28] a NNE model on a two-lane ring (one driven, the other undriven) was found to exhibit particle migration to the undriven region for smaller global densities and migration in the opposite sense for $\rho > 0.3$. Although a full explanation of the transport mechanism is not available, it appears [28] that diagonal strings of particles near the boundary between driven and undriven regions favor the transfer of particles from the former to the latter. Since the present study is concerned with macroscopic behavior, we defer further analysis of this question to future work.

From the macroscopic viewpoint, the driven and undriven regions correspond to systems coexisting under particle exchange. One therefore expects the stationary properties to be

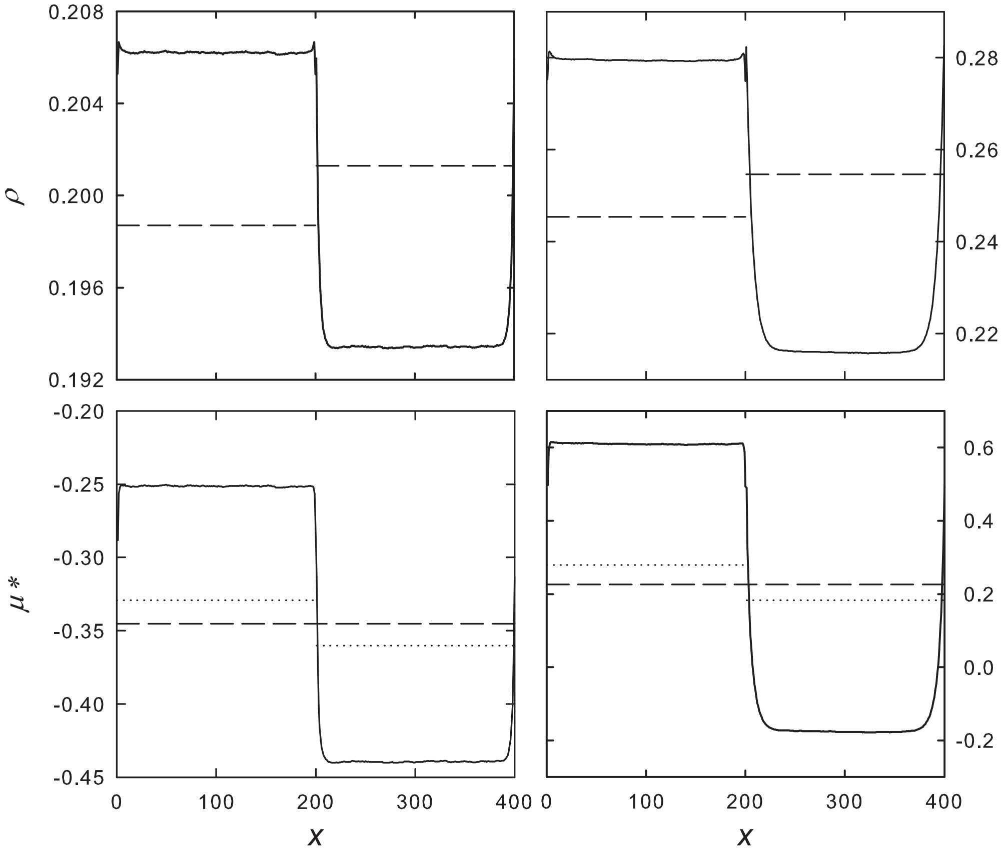

FIG. 4. Density (upper) and chemical potential (lower) profiles in the half-driven NNE model. Drive $D = 0$ for $x \leqslant 200$; $D = 1$ for $x > 200$. Global densities $\overline{\rho} = 0.2$ (left) and 0.25 (right). In the upper panels the dashed lines show the coexisting densities predicted by equating chemical potentials. In the lower panels the dashed lines show the expected uniform value of the chemical potential, and the dotted lines show the chemical potentials for the isolated systems, each at density $\overline{\rho}$.

predicted by SST, which it evidently does not. Is the failure due to limited system size? Studies using $L = 200$, 300, 400, and 800 yield essentially the same results, eliminating size as a possible explanation. Another possibility is that the exchange between the two regions must be weaker for SST to function, since, as noted above for pointwise exchange, as well as in Ref. [19], full agreement with the predictions of SST requires that we take the weak-exchange limit. Studies in which the acceptance probability for transfers between the two regions, p_r, is small, reveal essentially the same pattern as observed for $p_r = 1$. In the example shown in Fig. 6, for global density 0.22, the departure from the expected behavior is in fact somewhat greater for small values of p_r.

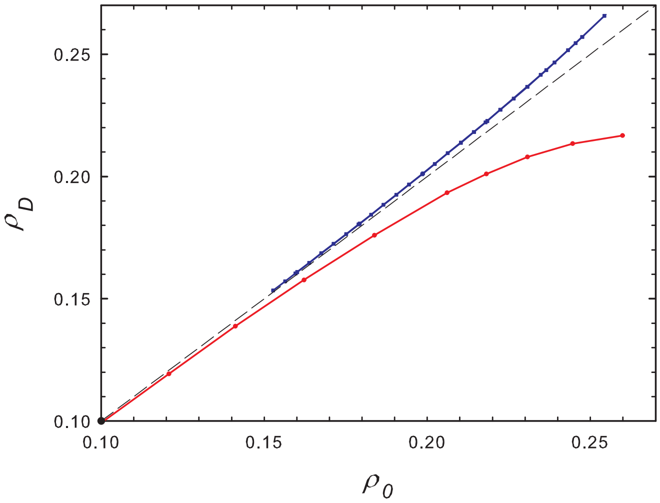

FIG. 5. (Color online) Coexisting bulk particle densities ρ_D and ρ_0, in driven and undriven regions, respectively, in the NNE model, as predicted by equating the chemical potentials in isolated systems (upper curve) and observed in simulations of the half-driven system (lower curve). Error are bars smaller than symbols. For purposes of comparison, the dashed line represents $\rho_D = \rho_0$.

B. NNE2 dynamics

I study the half-driven model with NNE2 hopping dynamics using simulation parameters similar to those used in the NNE case. Since the phase transition to sublattice ordering occurs for $\rho \simeq 0.35$ [26], the studies can be extended to higher densities than for NNE dynamics. Studies with $L = 200$ and 400 yield the same bulk values for ρ and μ^* to within uncertainty.

In contrast to the NNE case, under NNE2 dynamics the stationary density is higher in the driven region, as predicted by SST. The density profiles follow $\Delta\rho \sim e^{-x/\lambda}$, with λ ranging from near unity to about 3.0 in the nondriven region, as the bulk density varies from 0.25 to 0.34; in the driven region λ ranges from unity to 16.0 over this range of densities.

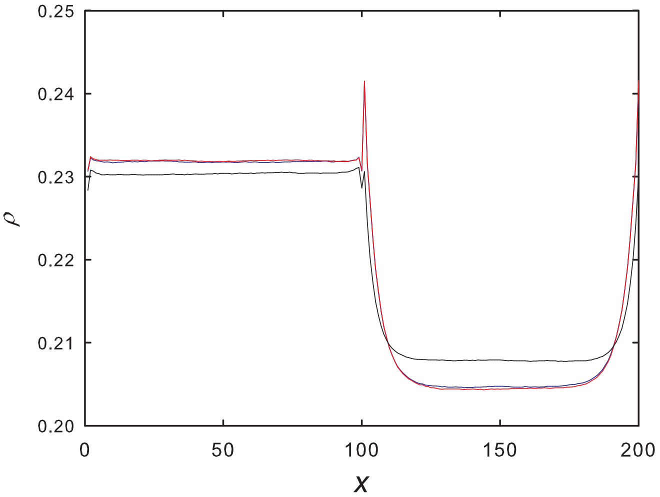

FIG. 6. (Color online) Density profiles in the half-driven NNE model with global density 0.22; drive $D = 0$ for $x \leqslant 100$; $D = 1$ for $x > 100$. Black: $p_r = 1$; blue: $p_r = 0.005$; red: $p_r = 0.002$.

The observed density and chemical potential profiles are again inconsistent with those expected on the basis of SST. As shown in Fig. 7, the bulk densities do not take their expected values, and the chemical potential profile is not uniform. Once again, the principle of equal chemical potentials in systems that coexist under particle exchange is violated. The general lack of agreement is evident in the comparison (Fig. 8) between predicted and observed densities in the driven and undriven regions. At lower global densities, ρ_D exceeds the value predicted using SST, while at higher global densities (above about 0.29) the trend reverses. (The difference $\rho_D - \rho_0 \propto \rho^2$ as the global density ρ tends to zero.) As in the NNE case, reducing the acceptance probability, p_r, for transfers between the driven and undriven regions only serves to enhance (slightly) the discrepancy between simulation and SST. Once again, the bulk values of ρ and μ^* in the driven and undriven regions agree with those found for the corresponding isolated systems, as shown in Fig. 9.

C. Conditions for stationarity and for a uniform chemical potential

It is worth contrasting the condition of (I) thermodynamic coexistence (spatially uniform chemical potential) with that (II) of a stationary density profile perpendicular to the drive. On the square lattice, condition I implies that the ratio of the probabilities of the two five-site clusters (a and b) shown in Fig. 10 be independent of position, whereas condition II simply requires that at each row j along the drive, the probabilities of clusters c and d be the same. The condition of uniform μ^* derives from the definition of chemical potential via exchange with a particle reservoir [19]. But since the driven lattice gas is not in contact with such a reservoir, there is no reason for condition I to apply in the presence of a nonuniform drive. Condition II does apply (else there would be a current perpendicular to the drive); it can be satisfied in a multitude of ways, depending on the details of particle fluxes in each row along the drive.

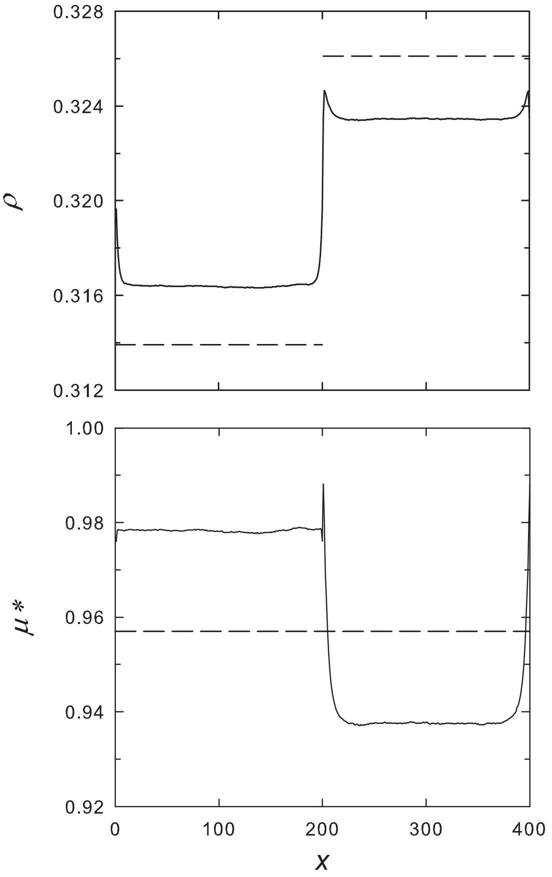

FIG. 7. Density (upper) and chemical potential (lower) profiles in the half-driven NNE2 model with global density $\overline{\rho} = 0.32$. Drive $D = 0$ for $x \leqslant 200$; $D = 1$ for $x > 200$. In the upper panel the dashed lines show the coexisting densities predicted by equating chemical potentials. In the lower panel the dashed line shows the expected uniform value of the chemical potential.

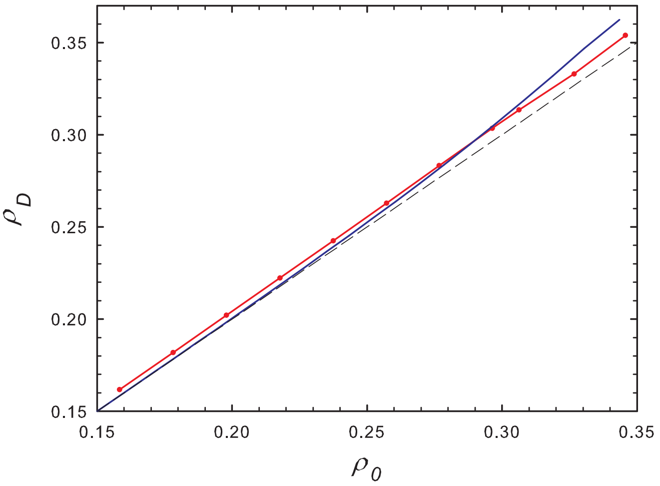

FIG. 8. (Color online) Coexisting bulk particle densities ρ_D and ρ_0, in driven and undriven regions, respectively, of the NNE2 model, as predicted by equating the chemical potentials in isolated systems (lower curve at left) and observed in simulation (upper curve at left). For purposes of comparison, the dashed line represents $\rho_D = \rho_0$.

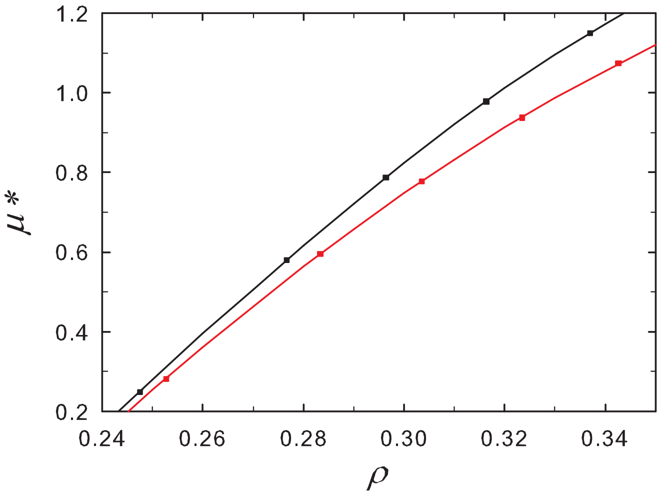

FIG. 9. (Color online) Points: Bulk chemical potential versus bulk density in driven (lower) and undriven (upper) regions of half-driven NNE2 model. The curves show the corresponding values for isolated systems. Error bars are smaller than symbols.

V. NONUNIFORM DENSITY, UNIFORM DRIVE

Having verified, in the preceding section, that the predictions of SST are strongly violated under a nonuniform drive, I turn in the present section to examples with a uniform drive, but a nonuniform particle density.

A. NNE2 lattice gas between hard walls

An equilibrium fluid, on- or off-lattice, typically exhibits a spatially varying density in the neighborhood of a hard repulsive wall. The chemical potential is nevertheless uniform. This observation motivates study of a *uniformly driven* lattice gas between hard walls. I study the NNE2 model on systems of $L \times L$ sites, with periodic boundaries (as always) along the drive and hard walls parallel to it, i.e., at rows $y = 0$ and $y = L + 1$. (In practical terms, transitions from $y = 1$ to $y = 0$, and from $y = L$ to $y = L + 1$, are simply prohibited.) As previously, sufficient time (in this case, 10^9 time units) is allowed for the system to attain the stationary state. Figure 11 compares typical density and chemical potential profiles in the equilibrium and fully driven ($D = 1$) systems. The density profiles are remarkably similar, exhibiting the familiar density enhancement adjacent to the walls. Despite the density variations, the equilibrium chemical potential profile is perfectly flat. In the driven system, by contrast, μ^* varies considerably.

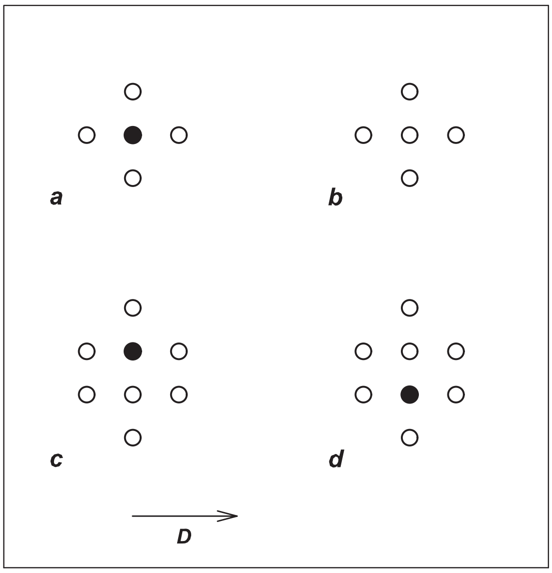

FIG. 10. Clusters on the square lattice. A uniform chemical potential requires that the ratio of the probabilities of clusters *a* and *b* be the same everywhere. A time-independent density profile perpendicular to the drive **D** requires that at each row parallel to **D**, the probabilities of clusters *c* and *d* be equal.

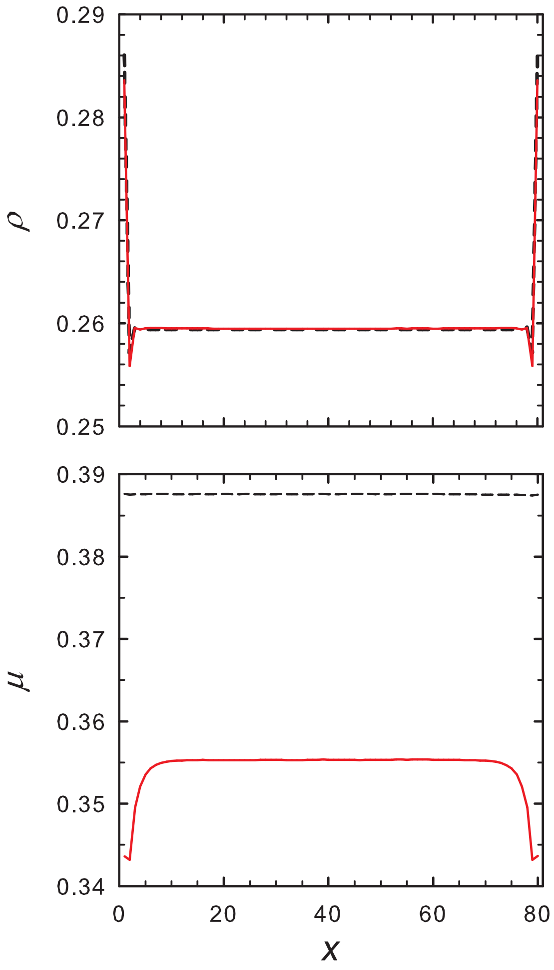

FIG. 11. (Color online) NNE2 lattice gas confined between hard walls parallel to the drive direction. Density profiles (upper) and chemical potential profiles (lower) in equilibrium (broken line) and under maximum drive (solid lines), for overall density $\rho = 0.26$.

B. NNE lattice gas with a row of slow bonds

As a further example of a spatially nonuniform system, I consider briefly the *uniformly driven* NNE model under periodic boundaries, but with *slow exchange* (hopping probability $p_r = 0.01$) between rows $y = L/2$ and $y = L/2 + 1$,

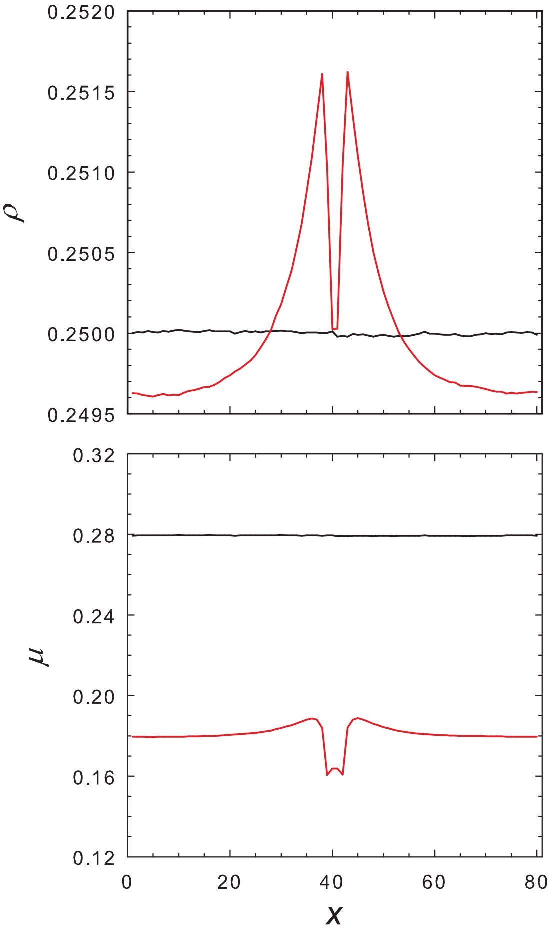

FIG. 12. (Color online) NNE lattice gas with periodic boundaries, with slow bonds (hopping probability $p_r = 0.01$) between rows $y = L/2$ and $y = L/2 + 1$. Density profiles (upper) and chemical potential profiles (lower) in equilibrium (flat profiles) and under maximum drive (nonuniform profiles) for overall density $\rho = 0.25$.

parallel to the drive (the slow bonds connecting these rows are oriented *perpendicular* to the drive). In equilibrium, such a nonuniform kinetics cannot affect stationary properties, since detailed balance is preserved. With or without a drive, each row of constant y coexists with neighboring rows, implying a uniform chemical potential. In the driven NNE system, nevertheless, the slow bonds cause significant variation of the density *and* chemical potential, as illustrated in Fig. 12.

VI. EXCHANGE BETWEEN SYSTEMS WITH IDENTICAL STEADY STATES

Consider two isolated, driven systems, A and B, of identical dimensions and having the same number of particles but with all transition rates in B equal to the corresponding rates in A multiplied by a common factor $q < 1$. Systems A and B possess identical stationary probability distributions on configuration space, since this distribution is invariant under a rescaling of time. When placed in contact, they should therefore coexist. This is verified (for both NNE and NNE2 dynamics) in the case of pointwise exchange for exchange rate p_r tending to zero.

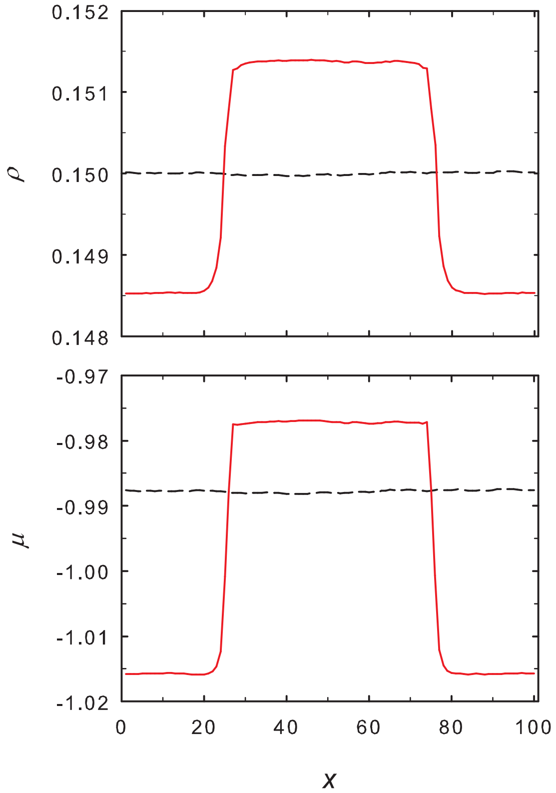

FIG. 13. (Color online) NNE lattice gas with all hopping rates reduced by $q = 0.5$ in the central region (see text). Density profiles (upper) and chemical potential profiles (lower) in equilibrium (dashed lines) and under maximum drive (solid lines) for overall density $\rho = 0.15$.

Consider next systems A and B in contact along an edge, as in previous examples. I study systems of $L \times L$ sites with periodic boundaries, in which transition rates in half the system are reduced by a factor q. Specifically, all rates of hopping *along* the drive are reduced in rows $y = L/4 + 1$ to $y = 3L/4$. Hopping rates *perpendicular* to the drive, from y to $y + 1$, are reduced in rows $y = L/4 + 1$ to rows $3L/4 - 1$, while for for hopping in the opposite sense (from y to $y - 1$) the reduction is imposed in rows $y = L/4 + 2$ to $y = 3L/4$. (In this way, the hopping rate from y to $y + 1$ is always equal to that from $y + 1$ to y, eliminating any intrinsic bias.) Although the subsystems in the inner and outer regions possess one and the same steady state when in isolation, they do not coexist under edgewise exchange in the presence of a drive: Under NNE dynamics, particles migrate from the fast to the slow region; under NNE2 dynamics migration occurs in the opposite sense. (Analogous migrations are observed in the half-driven systems described in Sec. IV: from driven to nondriven under NNE dynamics and vice versa.) Figure 13 shows typical stationary density and μ^* profiles for the NNE case.

VII. CONCLUSIONS

I test the predictive value of steady-state thermodynamics in athermal lattice gases subject to a nonuniform drive or other perturbations that provoke a nonuniform particle density. In the case of pointwise exchange (Sec. III), the predictions of SST are valid only in the limit of a vanishing exchange rate, $p_r \to 0$. For finite p_r the density profile is nonuniform and SST predictions are violated.

In studies of half-driven systems (Sec. IV), SST is found ineffective in predicting the coexisting particle densities of the driven and nondriven systems when they exchange particles across the interface, for both nearest-neighbor hopping (NNE dynamics) and nearest- and next-nearest hopping (NNE2 dynamics), regardless of the transfer probability p_r at the boundary. Of course, if we take p_r to zero in this situation, we obtain a pair of isolated systems separated by hard walls. As shown in Sec. V, the nondriven system then exhibits, as expected, a uniform chemical potential, but this is not the case under the drive.

The essential difference between the setup of Ref. [19], in which coexistence is attended by equality of the chemical potential, and the examples studied here, in which it is not, is the mode of particle transfer (global versus local). The global transfer scheme of Ref. [19], while useful in eliminating complicating effects of inhomogeneities, is not realizable in the laboratory. In the present study, by contrast, exchange is restricted to the region of contact between the subsystems The violation of SST is generally smaller under NNE2 dynamics, which features a longer range of particle motion. This is consistent with the observation that, extending the range of motion to include all sites, one would have *global* exchange, for which SST is in fact valid.

It is important to distinguish two classes of violations of SST. One class corresponds to inequalities of (or nonuniformities in) the chemical potential $\mu^* = \ln(\rho/\rho_{\rm op})$ in systems that coexist at stationarity. All of the violations of SST discussed here exhibit this feature; all are associated with nonuniform particle densities. Although there is no obvious candidate for a revised chemical potential (adding, e.g., some contribution that is identically zero in equilibrium), such an extended definition, that might yield, for example, a constant μ^* profile in a driven system between hard walls, appears to remain a logical possibility. This is a delicate question, since the definition of μ^*, based on the elementary principle of coexistence with a reservoir, functions perfectly for weak exchange between spatially uniform systems. Its redefinition (if possible) might therefore have to involve the local density gradient in the presence of a drive. Here it is well to recall that such details fall outside the usual notion of macroscopic thermodynamic variables.

Another class of violations, highlighted in Secs. IV and VI, involves pairs of systems that coexist in some situations (i.e., under global or pointwise weak exchange), but not in others, such as exchange along an edge. These inconsistencies arise *regardless of whether, or how, we define a chemical potential* and cannot be eliminated by its redefinition. They rather suggest the far more sweeping conclusion that SST only describes coexistence under vanishing exchange rates, between spatially uniform systems, and cannot be applied outside this limit. This would exclude, in particular, application of SST to nonuniform systems with a finite rate of particle exchange between distinct coexisting regions, as occurs, for example, in phase separation. The failure of SST in the simple context of driven lattice gases strongly suggests that the thermodynamics of nonequilibrium steady states has rather limited utility. Tests of SST in other model systems are planned for future work.

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[20] The Sasa-Tasaki (ST) rate for transfer of a particle from system A to system B depends exclusively on parameters associated with A and vice versa [16]. Imposing detailed balance, the ST rate for this transition takes the form $w_{\rm ST} = \epsilon \exp[\beta(\mu_A - \Delta E_A)]$, where E_A is the energy of interaction between the particle and its neighbors, and ϵ is an arbitrary rate factor. The ST expression can be seen as resulting from a very high energy barrier between

A and B; the particle first makes a transition from A to the barrier and from there to B. The transition rates used in the present study of athermal systems satisfy the ST condition intrinsically, since there are no changes in energy.

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