Sub-block order parameter in a driven Ising lattice gas using block distribution functions

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We investigate the order parameter of the standard Ising lattice gas and driven Ising lattice gas models. The sub-block order parameter is introduced to these conserved models as an order parameter using block distribution functions. We also introduce the sub-block order parameter of damage using the block distribution functions of damage. We measure the sub-block order parameters using the Metropolis and heat-bath rates. These order parameters work well for the non-equilibrium-conserved model as well as the equilibrium-conserved model. We obtain the critical exponent of order parameter $\beta=1/8$ for the standard Ising lattice gas and $\beta=1/2$ for a driven Ising lattice gas using the Metropolis and heat-bath rates.

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I. INTRODUCTION

Monte Carlo simulations play a major role in studying phase transitions and critical phenomena in statistical physics [1–10]. In this paper, Monte Carlo simulations have been carried out in order to investigate the order parameter of two conserved models: the standard Ising lattice gas model and its nonequilibrium cousin, the driven Ising lattice gas model [or the Katz-Lebowitz-Spohn (KLS) model [11]]. The essential difference between the conserved and nonconserved models is conservation of the order parameter. The two conserved models involve particles diffusing on a lattice, subject to an attractive nearest-neighbor interaction. The total number of particles is conserved. Due to the conservation of particles, the standard order parameter remains constant in two conserved models. It is thus fruitful to introduce a proper order parameter describing the dynamics of conserved models. We have introduced the sub-block order parameter based on block distribution functions.

In the statistical physics of many-body systems, it is a familiar concept to divide the system into "blocks" of a finite linear dimension L. This concept has been applied to understand the phase coexistence in the Ising lattice fluid and to estimate the critical exponents [6,7]. For the standard Ising lattice gas, the rate hopping to the unoccupied nearest-neighbor site is chosen to satisfy the detailed balance, with respect to Ising Hamiltonian in zero magnetic field. However, the KLS model involves an additional external force which acts on particles much like an "electric field" on (positive) charges. In the presence of an infinite external electric field and periodic boundary conditions, the particle-conserving irreversible dynamics does not reach an equilibrium state, but it develops the ordering which is very anisotropic with striplike configurations parallel to the electric field at low temperature [12,13]. We measure the sub-block order parameter using the Metropolis [14] and heat-bath rates [13,15]. The critical temperature and the critical exponent of order parameter are estimated using finite-size scaling of the sub-block order parameter and the sub-block order parameter of damage, respectively. The sub-block order parameter of damage is obtained using the damage spreading method [16]. For the standard Ising lattice gas, both the critical temperature and the critical exponent of the order parameter obtained from isotropic finite-size scaling do not depend on the transition rate. We apply anisotropic finite-size scaling to the KLS model. The critical exponent of the order parameter also does not depend on the transition rate, but the critical temperature does.

II. BACKGROUND

A. Models

The Hamiltonian of the standard Ising lattice gas model is given by

$$\mathcal{H} = -\phi \sum_{\langle i,j\rangle} \sigma_i \sigma_j, \tag{1}$$

where $\sigma_i=1$ for an occupied site, $\sigma_i=-1$ for an empty site, and ϕ for the binding energy.

The KLS model is a simple modification of the standard Ising lattice gas in which particles are driven by an external "electric field" $\mathcal{E}$. For the KLS model the transition rate is given by $w[\beta(\Delta\mathcal{H}+l\mathcal{E})]$, where $\mathcal{H}$ is the Hamiltonian of the standard Ising lattice gas and $l=(-1,0,+1)$ for jumps (along, transverse to, against) the drive $\mathcal{E}$, respectively. In the presence of an infinite "electric field" and periodic boundary conditions, the particle-conserving irreversible dynamics does not reach an equilibrium state because particles move endlessly along the closed strip.

B. Transition rates

The Metropolis and heat-bath rates are implemented to the standard Ising lattice gas and KLS models. The transition probability for the Metropolis rate [17] depends on the initial state and the final state, but the transition probability for the heat-bath rate [15] depends on the final state only. The heat-

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bath rate has been devised and implemented to the standard Ising lattice gas and KLS models [13].

C. Sub-block order parameter

There is no standard order parameter in the conserved system such as the standard Ising lattice gas and KLS models. We introduce the sub-block order parameter using block distribution functions. If we divide the conserved Ising lattice systems (the standard Ising lattice gas and KLS models) into blocks, above the critical temperature T_c, the distribution function of the local order parameter (block distribution function) has one highly likely local density (preferred local density) because the system is homogeneous. Below T_c the distribution function of the local order parameter has two highly likely local densities (preferred local densities, one positive ρ_+ and the other negative ρ_-) because the system is separated into the regions of particles and vacancies. These block distributions tend toward the Gaussian distribution centered around zero block (not sub-block) magnetization, so the spontaneous magnetization per spin, m, is equivalent to the average of two local preferred densities ρ_+ and ρ_-.

Thus we define the sub-block order parameter as follows:

$$m = \frac{\rho_+ - \rho_-}{2}. \tag{2}$$

Using the sub-block order parameter is the same kind of approach as the renormalization group [8,18], so that we can perform finite-size scaling for the sub-block parameter in different sub-blocks of the system.

D. Damage spreading method

The damage spreading was first studied for the theoretical biology in the context of genetic evolution [16]. In the damage spreading method, two different initial configurations are simulated with the same random number and the average damage between two different configurations—i.e., Hamming distance—is measured at every Monte Carlo step (MCS). The damage is 1 if two sites are different in the different configurations, or the damage is 0 if two sites are the same. Phase transitions and critical phenomena have been studied using the Monte Carlo damage spreading method for two-dimensional (2D) Ising [3,19,20], 3D Ising [21], and Potts [22] and Blume-Capel [23] models with various spin-flip dynamics (heat-bath, Glauber, and Metropolis). Although the damage spreading method for the nonconserved systems is well studied, this method has not been applied to the conserved system.

The damage is defined as

$$D(t) = \frac{1}{2N}\sum_i |O_i(t) - R_i(t)|, \tag{3}$$

where $\{O_i(t)\}$ is the original configuration, $\{R_i(t)\}$ is the replica configuration, and N is the number of sites. After creating an initial damage D_0 in the replica at $t=0$, we measure the damage. We will see that the initial damage D_0, initial configuration, and transition rate are all important.

We are interested in the sub-block damage because the zero-block damage does not work for the conserved system. In this paper, the local preferred damage density in the sub-block serves as a proper order parameter for the conserved system.

E. Finite-size scaling

For the isotropic system with linear dimension L, the correlation length ξ is given by

$$\xi \sim t^{-\nu}, \tag{4}$$

where $t=|\frac{T}{T_c}-1|$. The finite-size scaling form of the order parameter for a square lattice is given by

$$m = L^{-\beta/\nu}\tilde{m}(L^{1/\nu}t), \tag{5}$$

where the critical exponents of the standard Ising lattice gas are known as $\beta=1/8$ and $\nu=1$ [24,25].

For the anisotropic system, the correlation length $\xi_\parallel$ along the drive $\mathcal{E}$ and $\xi_\perp$ perpendicular to the drive $\mathcal{E}$ are given by

$$\xi_\parallel \sim t^{-\nu_\parallel} \quad \text{and} \quad \xi_\perp \sim t^{-\nu_\perp}, \tag{6}$$

respectively. The scaling form of the order parameter for the $L_\parallel \times L_\perp$ system is given by [26]

$$m(T_c, L_\parallel, L_\perp) = L_\parallel^{-\beta/\nu_\parallel}\tilde{m}(tL_\parallel^{1/\nu_\parallel}, S), \tag{7}$$

where the shape factor S is

$$S = L_\parallel^{\nu_\perp/\nu_\parallel}/L_\perp. \tag{8}$$

For the fixed shape factor S, the finite-size scaling form of the order parameter is given by

$$m(T_c, L_\parallel) = L_\parallel^{-\beta/\nu_\parallel}\tilde{m}(tL_\parallel^{1/\nu_\parallel}). \tag{9}$$

From the field theory [27,28], the critical exponents of the KLS model in two dimensions are given by $\beta=1/2$, $\nu_\parallel=3/2$, and $\nu_\perp=1/2$. The anisotropic finite-size scaling form with structure factor, serving as an order parameter, was studied by extending the exact field theory [29,30]. Previous works for the anisotropic finite-size scaling of the KLS model with drive $\mathcal{E}$ in the y direction are performed by simulations with structure factor $S(1,0)$, which serves as an order parameter with the Metropolis rate [26,29,30].

III. RESULTS

A. Sub-block finite-size scaling

The preferred local density of a sub-block serves as an order parameter. The sub-block order parameter is given by Eq. (2).

For the standard Ising lattice gas, we perform simulations on the system size with linear dimension $L=144$. Then we estimate the sub-block order parameter for the sub-blocks: $L^{\text{sub}}=36$, 24, 18, 16, 12, and 8. We find that the critical temperature of the standard Ising lattice gas does not depend on the transition rate: the heat-bath rate [Fig. 1(a)] and the Metropolis rate [Fig. 1(b)].

For the KLS model, we perform simulations on the system size $L_\parallel \times L_\perp = 432\times 48$. Two shape factors $S=0.25$ and

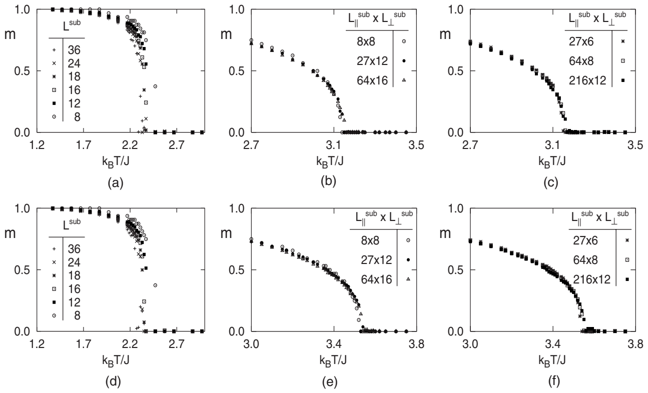

FIG. 1. Plots of the sub-block order parameter m for the standard Ising lattice gas model using (a) the Metropolis and (b) heat-bath rates. Plot of m for the KLS model with $S=0.25$ using (c) the Metropolis and (d) heat-bath rates and $S=0.50$ using (e) the Metropolis and (f) heat-bath rates. Simulations have been carried out with 2×10^6 MCS after discarding 8—10×10^6 MCS.

0.50 are available for a given system size. For $S=0.25$ [Figs. 1(c) and 1(d)], we estimate the sub-block order parameter for the sub-blocks: $L_{\parallel}^{\mathrm{sub}}\times L_{\perp}^{\mathrm{sub}}=64\times16$, 27×12, and 8×8. For $S=0.50$ [Figs. 1(e) and 1(f)], we estimate the sub-block order parameter for the sub-blocks: $L_{\parallel}^{\mathrm{sub}}\times L_{\perp}^{\mathrm{sub}}=216\times12$, 64×8, and 27×6. We find that the critical temperature of the KLS model does depend on the transition rate, but does not depend on the shape factor. The obtained value of the critical temperature T_c for the Metropolis rate in Figs. 1(c) and 1(e) is $T_c=3.15\pm0.05$ and for the heat-bath rate in Figs. 1(d) and 1(f) $T_c=3.55\pm0.05$.

Figures 2(a) and 2(b) show scaling plots of $\ln(mL^{\beta/\nu})$ as a function of $\ln(tL^{1/\nu})$ for the standard Ising lattice gas using (a) the Metropolis rate and (b) the heat-bath rate. For $T<T_c$, the critical exponent of the sub-block order parameter is obtained as $\beta=1/8$. This value is well consistent with the known results [24,25] and does not depend on the transition rate.

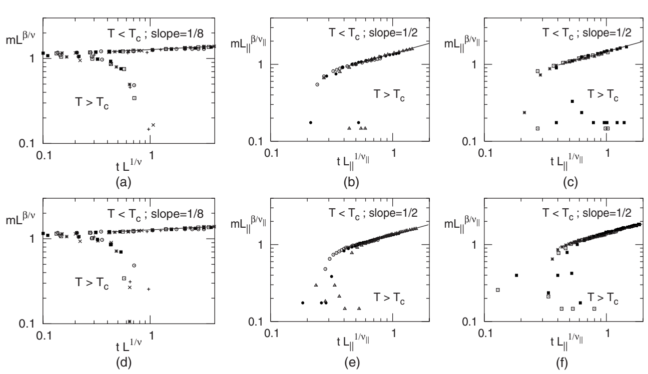

FIG. 2. Log-log plots of scaling function $mL^{\beta/\nu}$ as a function of scaling variable $tL^{1/\nu}$ for the standard Ising lattice gas model using (a) the Metropolis and (b) heat-bath rates. Log-log plots of scaling function $mL^{\beta/\nu_{\parallel}}$ as a function of scaling variable $tL^{1/\nu_{\parallel}}$ for the KLS model using the Metropolis rate for shape factor (c) $S=0.25$ and (e) $S=0.50$ and using the heat-bath rate for (d) $S=0.25$ and (f) $S=0.50$, respectively. All data symbols shown in these figures are the same as in Fig. 1.

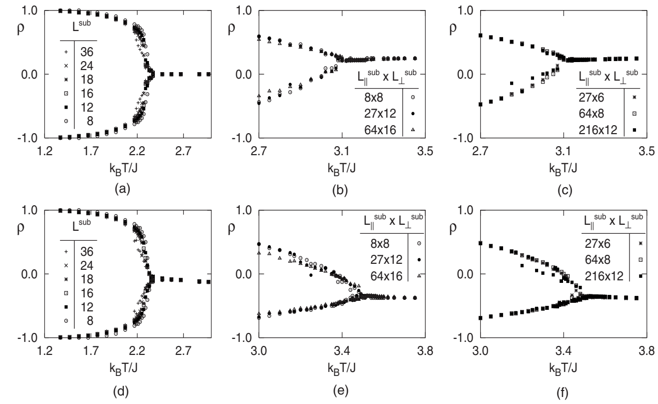

FIG. 3. Plots of the phase diagram of the preferred local densities ρ of damage in sub-blocks for the standard lattice gas model using (a) the Metropolis and (b) heat-bath rates. Plots of the phase diagram for the KLS model with $S=0.25$ using (c) the Metropolis and (d) heat-bath rates and with $S=0.50$ using (e) the Metropolis and (f) heat-bath rates, respectively. The upper branch uses $D_0\simeq1$ for the Metropolis and $D_0=1$ for the heat-bath rates. The lower branch uses $D_0=1/N$ for the Metropolis and heat-bath rates.

For the KLS model, we have various scaling plots of $\ln(mL_{\parallel}^{\beta/\nu_{\parallel}})$ as a function of $\ln(tL_{\parallel}^{1/\nu_{\parallel}})$ with two fixed shape factors $S=0.25$ [Figs. 2(c) and 2(d)] and $S=0.50$ [Figs. 2(e) and 2(f)]. From these scaling plots we obtain the critical exponent of the sub-block order parameter $\beta=1/2$. This value shows good consistency with the known results [26–30] and also does not depend on the transition rate the same as the standard Ising lattice gas does.

Using the sub-block finite-size scaling, we find that, for the standard Ising lattice gas, both critical temperature and the critical exponent do not depend on the type of transition rate. However, for the KLS model, the critical temperature depends on the type of transition rate and the critical exponent does not depend on the type of transition rate.

B. Sub-block damage finite-size scaling

In our simulations two kinds of initial damage are chosen for the standard Ising lattice gas and KLS models using the Metropolis and heat-bath rates.

Type I. Original and replica spin configurations are identical except one site, so initial damage $D_0=1/N$ for the Metropolis and heat-bath rates.

Type II. Original configuration is exactly opposite to replica spin configuration, so $D_0\simeq1$ for the Metropolis rate and $D_0=1$ for the heat-bath rate.

The system sizes and sub-block sizes used for the sub-block damage finite-size scaling are identical to those for the sub-block finite-size scaling in Sec. III A.

Figure 3 shows the phase diagrams of two models with two preferred local damage densities ρ_+ and ρ_-, where ρ_+ is the preferred local damage density estimated from type-II initial damage and ρ_- from type-I initial damage. For the standard Ising lattice gas, the phase diagram is symmetric about zero density, but for the KLS model it is asymmetric about nonzero density. Above the critical temperature T_c, ρ_+ has the same value of ρ_-. Below T_c, ρ_+ and ρ_- are different.

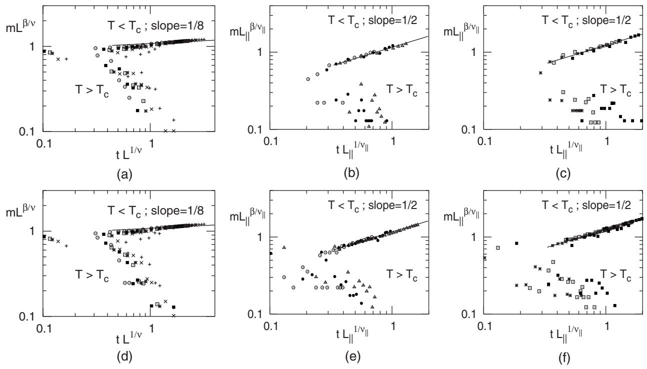

FIG. 4. Log-log plots of scaling function $mL^{\beta/\nu}$ as a function of scaling variable $tL^{1/\nu}$ for the standard Ising lattice gas model using (a) the Metropolis and (b) heat-bath rates where m is the sub-block order parameter of damage. Log-log plots of scaling function $mL^{\beta/\nu_\parallel}$ as a function of scaling variable $tL^{1/\nu_\parallel}$ for the KLS model using the Metropolis rate for shape factor (c) $S=0.25$ and (e) $S=0.50$ and using the heat-bath rate for (d) $S=0.25$ and (f) $S=0.50$, respectively. All data symbols shown in these figures are the same as in Fig. 3.

From Figs. 3(a) and 3(b) we observe that T_c for the Metropolis and heat-bath rates are identical. However, for the KLS model, the critical temperature does depend on a transition rate but does not depend on the shape factor. The obtained value of T_c for the Metropolis rate in Figs. 3(c) and 3(e) is $T_c=3.05\pm0.05$ and for the heat-bath rate in Figs. 3(d) and 3(f) $T_c=3.45\pm0.05$.

Using two preferred local damage densities ρ_+ and ρ_-, we can construct the sub-block order parameter of damage in the same manner as the sub-block order parameter in Eq. (2). We can apply the same finite-size scaling as the sub-block order parameter. For the standard Ising lattice gas, Figs. 4(a) and 4(b) show scaling plots for the Metropolis and heat-bath rates, respectively. The obtained critical exponent $\beta=1/8$ is consistent with the known value [24,25] and also does not depend on the transition rate the same as the sub-block order parameter does.

The rest of Fig. 4 shows scaling plots for the KLS model with two fixed shape factors $S=0.25$ [Figs. 4(c) and 4(d)] and $S=0.50$ [Figs. 4(e) and 4(f)]. We obtain the critical exponent of the sub-block order parameter of damage $\beta=1/2$ which is also consistent with the known value [26–30]. This value does not depend on both the shape factor and transition rate.

IV. CONCLUSIONS

The critical properties of the equilibrium-conserved model (the standard Ising lattice gas) and the non-equilibrium-conserved model (the KLS model) have been studied using the sub-block and sub-block damage finite-size scalings with two different transition rates: the Metropolis and heat-bath rates.

We apply the sub-block order parameter and the sub-block order parameter of damage for two conserved models: the standard Ising lattice gas and KLS models. These order parameters work very well for the equilibrium-conserved model (the standard Ising lattice gas model) as expected. We then show that these order parameters also work well for the nonequilibrium model (the KLS model).

By applying either the sub-block or sub-block damage finite-size scaling to the KLS model, we obtain the critical exponents of order parameter $\beta=1/2$ which is in good agreement with the field-theoretical results [26–30]. This value does not depend on the type of transition rate. The critical temperature, however, depends on the transition rate. The value of critical temperature using the heat-bath rate is always larger than that using the Metropolis rate, due to higher transition probability for all possible energy changes. The critical temperature for the standard Ising lattice gas model is always lower than for the KLS model. This effect is mediated by the anisotropy of correlation in the presence of an external field [11,12]. The obtained value of critical temperature ($T_c=3.15\pm0.05$) is well comparable with the previous results [12] obtained by the dynamic mean-field theory (MFT): $T_c\approx3.206$ (for pair MFT) and 3.134 (for square MFT).

In summary, we have studied the sub-block order parameter in the driven Ising lattice gas using block distribution functions. All our results support the suggestion that the sub-block order parameter can be used as an order parameter for the non-equilibrium-conserved model as well as the equilibrium-conserved model. We also find that the sub-block order parameter of damage is also well implemented for both conserved models.

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