Inequivalence of dynamical ensembles in a generalized driven diffusive lattice gas

Muktish Acharyya,[1,*] Abhik Basu,[2,†] Rahul Pandit,[2,‡] and Sriram Ramaswamy[2,‡]
[1]*Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore 560064, India*
[2]*Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012, India*
(Received 13 August 1999)

We generalize the driven diffusive lattice gas model by using a combination of Kawasaki and Glauber dynamics. We find via Monte Carlo simulations and perturbation studies that the simplest possible generalization of the equivalence of the canonical and grand-canonical ensembles, which holds in equilibrium, does not apply for this class of nonequilibrium systems.

PACS number(s): 05.40.−a, 05.70.Ln

For statistical systems in thermodynamic equilibrium, the equivalence of different ensembles in the thermodynamic limit is a well-established result [1]. Does this have an analog in driven systems that display nonequilibrium steady states and transitions between them? Perhaps not, in general; but it is important to investigate when, if at all, such an analog might exist. One aspect of this problem has been studied in Ref. [2] in the context of a Gallavotti-Cohen-type symmetry in the large-deviation functional for driven stochastic systems such as a driven diffusive lattice gas (DDLG). We have studied another aspect of this problem in the context of a *generalized* DDLG, which is one of the simplest driven models in statistical mechanics with a transition between different nonequilibrium steady states. We begin by recalling that the conventional DDLG (see below and Ref. [3]) uses number-conserving (Kawasaki) dynamics [4] to update particle positions; i.e., it is the analog of the canonical ensemble in equilibrium. To develop a grand-canonical analog we generalize the DDLG to include a chemical potential μ and a μ-dependent fraction of updates that use nonconserving (Glauber) dynamics [4]; the remaining fraction of updates use Kawasaki dynamics. We show the following: (1) our generalized DDLG is ideally suited to examining the simplest nonequilibrium analog of the equivalence of canonical and grand-canonical ensembles; (2) even in this simple driven system, the canonical and grand-canonical ensembles are *not equivalent*. We arrive at this result by using Monte Carlo simulations to study our DDLG and perturbation theory to investigate a continuum version of it. We end with some remarks about the relevance of our work to studies of phase coexistence in sheared mesogenic fluids [5].

It is useful to begin with a recapitulation of some elementary facts: The DDLG is based on a latttice-gas model in which the occupation variables n_i assume the values 1 or 0 depending on whether a particle is present or not at the site i. Such a model is simply related to an Ising model [6] defined in terms of the spin variables $S_i \equiv (2n_i - 1)$ by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i , \tag{1}$$

where the exchange coupling J and the magnetic field H are related, respectively, to the pair potential V and the chemical potential μ of the lattice gas, and $\langle ij \rangle$ are nearest-neighbor pairs of sites on a d-dimensional hypercubic lattice (we use a two-dimensional square lattice in our numerical studies). If $J>0$, model (1) is ferromagnetic and its lattice-gas analog has an attractive interparticle interaction. The equilibrium phase diagram of model (1) is well known: In the temperature T and H plane there is a first-order phase boundary at $H=0$ along the line $0 \leqslant T < T_c(d)$, which ends in a critical point at $T=T_c(d)$; this first-order boundary shows up as a region of two-phase coexistence in a T-M phase diagram, where the magnetization M is the Ising analog of the lattice-gas density ρ; constant-M and constant-H ensembles are the analogs of the canonical and grand-canonical ensembles (we will use Ising-model and lattice-gas terminology interchangeably in this paper). As noted before, these ensembles are equivalent [7] and one can use standard thermodynamic relations to go from one to the other. In particular, to obtain the coexistence curve in the T-M phase diagram from the first-order boundary in the T-H phase diagram, we merely have to find the jump in the magnetization across this phase boundary at all values of $T < T_c(d)$.

In the conventional DDLG, $H=0$ in model (1), the magnetization M is fixed, since Kawasaki spin exchange is used in Monte Carlo updates, and a nonequilibrium steady state is maintained as follows: An ''electric field'' $\mathbf{E}$ is applied; this forces all particles (assumed identically charged) to move along its direction $\boldsymbol{l}$; periodic boundary conditions are used in this direction. In Monte Carlo simulations, one uses the Metropolis algorithm [8] with a transition probability $\mathrm{Min}[1, e^{-\beta(\Delta\mathcal{H} + \boldsymbol{l}\cdot\mathbf{E})}]$, where $\Delta\mathcal{H}$ is the change in energy because of the Kawasaki spin exchange and $\beta \equiv (k_B T)^{-1}$, with k_B the Boltzmann constant. Note that the field $\mathbf{E}$ favors particles moving along its direction, disfavors the opposite, and does not affect jumps in transverse directions. Extensive studies [3] have shown that this DDLG exhibits two-phase

*Present address: Theoretische Physik Universität-Duisburg, D-47048 Duisburg, Germany.
†Also at Poorna Prajna Institute of Scientific Research, Bangalore, India.
‡Also at Jawaharlal Nehru Institute for Advanced Scientific Research, Bangalore, India.

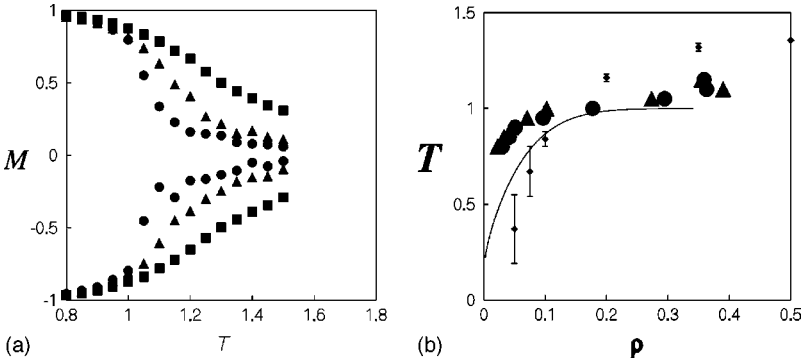

FIG. 1. (a) The variation of the magnetization M with the temperature T for our generalized DDLG with $L=32$, $E=\infty$, and the magnetic field $H=\pm 0.05$ (squares), $H=\pm 0.02$ (triangles), and $H=\pm 0.01$ (circles). (b) First-order phase-coexistence curves for the conventional DDLG (small diamonds) [9], for our generalized DDLG (circles for $L=16$ and triangles for $L=32$), and for the two-dimensional Ising model in equilibrium (solid line). Note that $\rho=(1+M)/2$.

coexistence for $T<T_c^K(d,E)$, where $E\equiv|\mathbf{E}|$ and the superscript K stands for Kawasaki to help us to distinguish this critical temperature from the one we obtain below for our generalized DDLG. For the infinitely biased case, $E=\infty$, e.g., $T_c^K(d=2,E=\infty)\simeq 1.35T_c^K(d=2,E=0)$, where $T_c^K(d=2,E=0)$ is just the Onsager critical temperature for the two-dimensional Ising model in equilibrium. Critical exponents have been obtained for $E>0$ [3] and one study [9] has investigated the coexistence curve in the T-M plane.

We have generalized the DDLG by introducing Glauber spin-flip moves [10] in addition to the Kawasaki spin-exchange moves mentioned above. We choose the ratio f_G of the number of these Glauber moves to the total number of moves to be proportional to H^2. Thus, as $H\to 0$, $f_G\to 0$, in the simplest analytic way that is even in H. By virtue of these Glauber moves our generalized DDLG does not conserve the number of particles and thus provides a suitable extension of the grand-canonical ensemble for this nonequilibrium system. We might think naively that, as $H\to 0$, we regain the conventional DDLG with only Kawasaki updates. However, we must exercise caution here for there is some subtlety in the order in which limits are taken: since $f_G\sim H^2\to 0$ as $H\to 0$, we must run a Monte Carlo simulation for a time τ_{SS} at least $\sim H^{-2}$ so that the system experiences a large enough number of Glauber moves and attains its true steady state; i.e., we must take the $\tau_{SS}\to\infty$ limit *before* we take $H\to 0$ [just as in equilibrium studies we take the thermodynamic limit (system size $L\to\infty$) before we take the $H\to 0$ limit while calculating the magnetization].

In our Monte Carlo simulations we use a square lattice of side L. In most of our studies $E=\infty$ and is applied along the $+x$ direction. Thus jumps along this direction are always accepted, those in the $-x$ direction are forbidden, and jumps along the $\pm y$ directions are not affected by $\mathbf{E}$. We choose at random the spin that has to be updated, measure time in units of Monte Carlo steps per spin (MCS), and use random initial conditions. At each set of values of H and T we wait for the system to reach a statistical steady state, characterized by a steady mean value of the magnetization per site $[M(H,T)\equiv(1/L^2)\Sigma_i S_i]$, and then obtain data for average values of the quantities we measure. We obtain the coexistence curve in our dynamical grand-canonical ensemble by determining $M(H,T)$ both as $H\uparrow 0$ and $H\downarrow 0$, for $T<T_c^{GK}$, where the superscript GK indicates that this is the critical temperature for our generalized DDLG, which uses Glauber *and* Kawasaki spin updates. Curves of M versus T are shown for different values of H in Fig. 1. We use such curves to obtain the $H\uparrow 0$ and $H\downarrow 0$ limits of $M(T,H)$ and thence the coexistence curve of Fig. 1(b) (we show only the left half of this curve since it is symmetrical about $M=0$ or $\rho=1/2$).

Our coexistence curves for $L=16$ and $L=32$ [Fig. 1(b)] are within error bars of each other, so finite-size corrections to our results are not significant except very near the critical point at $\rho=1/2$, $T=T_c^{GK}\simeq 1.1$. For comparison we have shown the coexistence curve obtained in Ref. [9] for the conventional DDLG, in which only Kawasaki updates are used; we also show the Onsager result for the two-dimensional Ising model in equilibrium. Figure 1(b) illustrates two important features: (1) $T_c^{GK}<T_c^K$ and the coexistence curve for our generalized DDLG is distinctly different from that for the conventional DDLG [9]; the former bows out to higher temperatures near T_c^{GK}, but then crosses the latter and subsequently lies below it. (2) The coexistence curve for our generalized DDLG is quite close to Onsager's result for the two-dimensional Ising model in equilibrium [3]. We give a perturbative justification below. However, before we do this, it is useful to try to understand these results qualitatively. In our generalized DDLG, we approach the coexistence curve by taking the limits $H\uparrow 0$ or $H\downarrow 0$. Thus, if $T<T_c^{GK}$, most spins assume the value $\mathrm{sgn}(H)$, and there are no macroscopically large interfaces as in the conventional DDLG. Consequently, the electric field $\mathbf{E}$, which is the source of the nonequilibrium behavior here, has a smaller effect in our generalized DDLG than it does in the conventional DDLG. This might well be the reason for the proximity of our coexistence curve to that of the two-dimensional Ising model in equilibrium.

To obtain a more detailed understanding of our Monte Carlo results, we have developed a Langevin or time-dependent Ginzburg-Landau (TDGL) model for our generalized DDLG. This is a simple extension of the Langevin model for the conventional DDLG [3]; since our purpose is merely to illustrate the phase-coexistence issues mentioned above, we restrict ourselves to a model in which all anisotropies, other than the driving electric field, are dropped. The Langevin equation for our model is

$$\frac{\partial\psi}{\partial t}=-\Gamma_0 H^2\left(\lambda\psi-H+\frac{u}{3!}\psi^3-c\nabla^2\psi\right)+E\partial_x\psi^2 + \left(\lambda\nabla^2\psi+\frac{u}{3!}\nabla^2\psi^3+c\nabla^4\psi\right)+\eta_1+\eta_2, \qquad (2)$$

where $\lambda\sim(T-T_c^{GK})$ is negative in the ordered phase, and $\psi\equiv\phi+M_0$, with M_0 the mean-field magnetization given by $\lambda M_0+(u/3!)M_0^3=H$. As in our lattice-gas model, the ki-

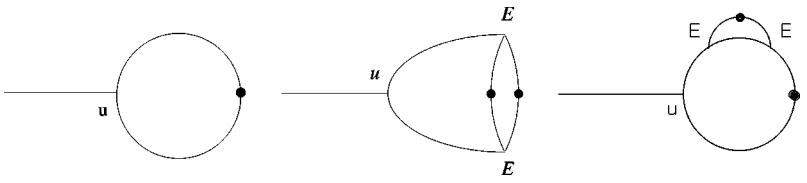

FIG. 2. Diagrams that contribute to the magnetization $M=\langle\psi\rangle$ to $O(u,E^2)$ for model (2). Lines represent response functions and lines with a filled circle correlation functions. Vertices marked with a u have a factor of $uH^2/2$ associated with them; those with an E have a factor iE.

netic coefficients in this Langevin equation are such that the order parameter ψ is conserved if $H=0$, and terms that lead to a violation of this conservation are proportional to H^2. The two noise terms η_1 and η_2 have zero mean and $\langle\eta_1(\mathbf{k},t)\eta_1(\mathbf{k}',t')\rangle=2\Gamma_0 H^2 k_B T\delta(\mathbf{k}+\mathbf{k}')\delta(t-t')$ and $\langle\eta_2(\mathbf{k},t)\eta_2(\mathbf{k}',t')\rangle=2k^2 k_B T\delta(\mathbf{k}+\mathbf{k}')\delta(t-t')$, where $\mathbf{k}$ and $\mathbf{k}'$ are wavevectors, $k\equiv|\mathbf{k}|$ and t and t' are times. The variances of the noise terms are chosen such that, in the long-time limit, the Boltzmann distribution obtains if $E=0$. Since the current $\mathbf{j}_E$ produced by $\mathbf{E}$ must vanish if no holes or no particles are present locally, we make the simplest choice that satisfies these constraints, namely, $\mathbf{j}_E=(1-\psi^2)\mathbf{E}$, which leads [3] to the term $E\partial_x\psi^2$ in our Langevin equation with the spatial derivative along $\mathbf{E}$ (chosen to be parallel to the x axis).

We now calculate $M\equiv\langle\psi\rangle$ perturbatively to $O(u,E^2)$ in the limits $t\to\infty$ and $H\to 0$. The diagrams in Fig. 2 contribute to this order. Thus, to $O(u,E^2)$

$$M=M_0+uM_0k_BTa_1+uE^2M_0(k_BT)^2a_2+uE^2M_0(k_BT)^2a_3, \tag{3}$$

where

$$a_1=-\frac{1}{2\lambda}\int\frac{d^2q}{-2\lambda+cq^2},$$

$$a_2=-\frac{1}{\lambda}\int\frac{d^2qd^2q_1}{-2\lambda q^2+cq^4}\,\frac{q_1^2}{-2\lambda q_1^2+cq_1^4-2\lambda(q-q_1)^2+c(q-q_1)^4}\,\frac{q_x^2}{-2\lambda+cq_1^2}\,\frac{1}{-2\lambda+c(q-q_1)^2},$$

$$a_3=-\frac{1}{2\lambda}\int\frac{d^2qd^2q_1q_x(q_{1x}-q_x)}{-2\lambda q^2+cq^4}\,\frac{1}{-2\lambda+cq_1^2}\,\frac{1}{-2\lambda+cq^2}\,\frac{1}{-2\lambda q^2+cq^4-2\lambda q_1^2+cq_1^4-2\lambda(q-q_1)^2+c(q-q_1)^4} \tag{4}$$

come from the loop integrals in Fig. 2; in order to compare with our lattice simulations we set the spatial dimension $d=2$.

The Langevin equation for the conserved case follows from Eq. (2) with $H=0$. We set $\psi=\phi+M$, where, at the end of the calculation, we will find that $M=M_0$, to the lowest order in u. Hence

$$\frac{\partial\phi}{\partial t}=\lambda\nabla^2\phi+\frac{u}{3!}\nabla^2\phi^3+\frac{u}{2}M^2\nabla^2\phi+\frac{u}{2}M\nabla^2\phi^2-c\nabla^4\phi+EM\partial_x\phi^2+\eta_2. \tag{5}$$

The term $2EM\partial_x\phi$ has been eliminated by a Galilean shift. We calculate correlation functions by using the dynamic generating functional [11]

$$J_c[\phi,\phi']=-\int dtd^2x\,\hat{\phi}\nabla^2\hat{\phi}+i\int dtd^2x\left(\left[\frac{\partial}{\partial t}-\lambda\nabla^2\phi-\frac{u}{3!}\nabla^2\phi^3-\frac{u}{2}M^2\nabla^2\phi-\frac{u}{2}M\nabla^2\phi^2-c\nabla^4\phi-E\partial\phi^2\right]\hat{\phi}+\hat{\phi}\nabla^2\phi\right), \tag{6}$$

where $\hat{\phi}$ is the Martin-Siggia-Rose conjugate variable [12]. Order-parameter conservation implies that $\phi(x,t)$ cannot respond to a spatially uniform magnetic field. In the two-phase regime phase separation proceeds via the formation of strips of up and down spins with the interfaces between these strips aligned, on average, parallel to $\mathbf{E}$ [3]. Thus the coupling to the field has the form $\int dtd^2x\hat{\phi}\nabla^2h(x_\perp)$ in the dynamical functional where the subscript $\perp$ denotes the direction perpendicular to E. As in Ref. [3] the equation of state is

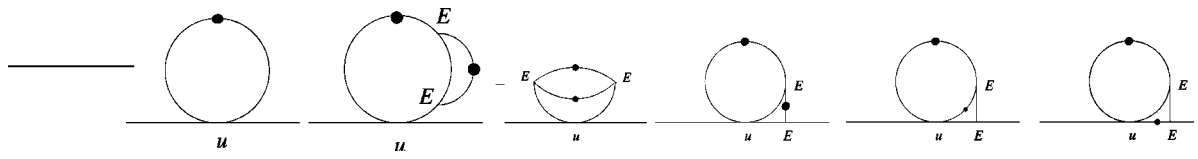

FIG. 3. Diagrams contributing up to $O(u)$ and $O(uE^2)$ to Γ^{11}.

$$h=\frac{\partial}{\partial k_\perp^2}\frac{\delta}{\delta\hat{\phi}}\Gamma[\psi,\hat{\phi}]|_{\mathbf{k}=\mathbf{0},\hat{\phi}=0,\psi=M}$$

$$=\frac{\partial}{\partial k_\perp^2}\frac{\delta}{\delta\hat{\phi}}\Gamma[\phi,\hat{\phi}]|_{\mathbf{k}=\mathbf{0},\hat{\phi}=0,\phi=0}, \tag{7}$$

where Γ is the vertex generating functional. A functional Taylor expansion of Γ about $\psi(q)=M\delta(q)$ yields

$$\Gamma[\phi,\hat{\phi}]=\sum_{n1=0,n2=0}^{\infty}\frac{1}{n_1!}\frac{1}{n_2!}\times\int d^2q_1\ldots d^2q_{n_1}d^2\tilde{q}_1\ldots d^2\tilde{q}_{n_2}\times[\phi(q_1)+M\delta(q_1)][\phi(q_2)+M\delta(q_2)]\ldots\phi(q_{n_1})\hat{\phi}(\tilde{q}_1)\ldots\hat{\phi}(\tilde{q}_{n_2})\times\Gamma^{n_1n_2}(q_1,\ldots,q_{n_1},\tilde{q}_1,\ldots,\tilde{q}_{n_2}). \tag{8}$$

If we are only interested in the spontaneous magnetization we set

$$h=0=\frac{\partial}{\partial k_\perp^2}\frac{\delta}{\delta\hat{\phi}(k)}\Gamma[\phi,\hat{\phi}]|_{\phi=M,\hat{\phi}=0}. \tag{9}$$

By retaining terms up to $O(M^3)$ we get

$$\frac{\partial}{\partial k_\perp^2}\left[M\Gamma^{11}+\frac{M^2}{2}\Gamma^{21}+\frac{M^3}{3!}\Gamma^{31}\right]=0, \tag{10}$$

which, when expanded to $O(u,E^2)$, yields

$$\begin{aligned}M&=\sqrt{\frac{-3!\lambda}{4}}[1+uk_BTb_1+uE^2b_2(k_BT)^2b_3\\&\quad+uE^2(k_BT)^2b_3+uE^2(k_BT)^2(\Delta_1+\Delta_2+\Delta_3)]\\&=M_0[1+uk_BTb_1+uE^2b_2(k_BT)^2b+uE^2(k_BT)^2b_3\\&\quad+uE^2(k_BT)^2(\Delta_1+\Delta_2+\Delta_3)],\end{aligned} \tag{11}$$

where, as for the case of our generalized DDLG, the mean-field magnetization $M_0=\sqrt{-3!\lambda/4}$, and b_1,b_2,b_3 and Δ are the loop integrals in Fig. 3, To this order we can set $M=M_0$ in the loop integrals. Hence we obtain $b_1=a_1$, $b_2=a_2$, $b_3=a_3$ and

$$\Delta_1=-\frac{1}{\lambda}\int\frac{d^2qd^2q_1}{-2\lambda q^2+cq^4-2\lambda(q+q_1)^2+c(q+q_1)^4-2\lambda q_1^2+cq_1^4}\frac{1}{-2\lambda q_1^2+cq_1^4}\frac{1}{-2\lambda+cq^2}\frac{q_{1x}(q_x+q_{1x})}{-2\lambda+cq_1^2},$$

$$\Delta_2=\frac{1}{2\lambda}\int\frac{d^2qd^2q_1}{-2\lambda q^2+cq^4-2\lambda(q+q_1)^2+c(q+q_1)^4-2\lambda q_1^2+cq_1^4}\frac{1}{-2\lambda q_1^2+cq_1^4}\frac{1}{-2\lambda+cq^2}\frac{q_{1x}^2}{-2\lambda+c(q+q_1)^2}, \tag{12}$$

$$\Delta_3=\frac{1}{2\lambda}\int\frac{d^2qd^2q_1}{-2\lambda q^2+cq^4-2\lambda(q+q_1)^2+c(q+q_1)^4-2\lambda q_1^2+cq_1^4}\frac{1}{-2\lambda q_1^2+cq_1^4}\frac{1}{-2\lambda+cq^2}\frac{q_{1x}(q_x+q_{1x})}{-2\lambda+cq_1^2}.$$

Notice that sum of the diagrams contributing to Γ^{31} and Γ^{21} to $O(uE^2)$ vanish (Fig. 4). This is a consequence of the invariance of our TDGL equations under $\mathbf{r}\to\mathbf{r}-\mathbf{E}t$ with $\phi\to\phi-1/(2M)$.

We now compare our TDGL results for the magnetizations of the generalized DDLG and conserved cases. We find that there is an extra contribution from the last three diagrams $\Delta_1,\Delta_2,\Delta_3$ in the latter; this is positive definite so $|M_K|>|M_{GK}|$. Of course if $E=0$ both are the same as they must be by virtue of the equivalence of ensembles in equilibrium. Our analytical results agree qualitatively with our Monte Carlo results for $0.2\lesssim\rho\lesssim0.4$ where the conventional DDLG coexistence curve lies above the one for our generalized DDLG (i.e., at a fixed value of $T,\rho_K>\rho_{GK}$ or, equivalently, $|M_K|>|M_{GK}|$); further away from this regime we must include higher-order terms in our functional Taylor expansion. In particular, we believe such terms are required to understand the crossing of the two coexistence curves in Fig. 1 for $\rho\lesssim0.2$. Note also that quantitative agreement between our analytical and numerical results is not expected at criticality since our one-loop approximation can only yield mean-field exponents.

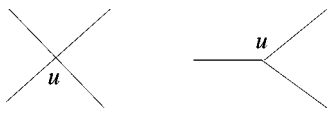

FIG. 4. Diagrams contributing up to $O(u)$ to Γ^{31} and Γ^{21}.

In conclusion, then, we have shown that the simplest generalizations of grand-canonical and canonical ensembles are not equivalent for our generalized DDLG. Our study, though carried out on a very simple model, has important lessons for work on phase coexistence in systems such as sheared nematogenic fluids [5]. Such studies have also found that constant-shear-rate and constant-stress ensembles yield different phase-coexistence boundaries. However, while determining such boundaries, the ''chemical potentials'' (defined as in equilibrium, i.e., as the derivative of a ''free energy'' with respect to particle density) in the two coexisting phases are equated. The lesson from our work is that this is valid only in the limit of very low shear rate (or E in our example); really we must equate $\partial\Gamma\partial\phi$ in the two coexisting phases;

this will yield the equality of the chemical potentials in equilibrium but will have corrections at finite E [of $O(uE^2)$ to lowest order].

Note added in proof. The *critical* behavior of a DDLG with mixed kinetics (but different from our model in detail) has been studied numerically by J.-S. Wang, K. Binder, and J. L. Lebowitz, J. Stat. Phys. **56**, 783 (1989) and analytically by K. E. Bassler and B. Schmittmann, Phys. Rev. Lett. **73**, 3343 (1994). We thank B. Schmittmann for bringing this to our notice.

We thank A. Sain for discussions, SERC (IISc) and JNCASR (India) for computational resources, and CSIR (India) for financial support.

[1] D. Ruelle, *Statistical Mechanics* (Benjamin, Reading, MA, 1969).

[2] J.L. Lebowitz and H. Spohn, e-print cond-mat/9811220.

[3] R. K. P. Zia and B. Schmittman, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J.L. Lebowitz **17** (Academic, New York, 1995), Vol. 17.

[4] K. Kawasaki, Phys. Rev. **148**, 375 (1966).

[5] P. D. Olmsted and C.-Y. D Lu, Phys. Rev. E **56**, R55 (1997).

[6] K. Huang, *Statistical Mechanics* (Wiley Eastern, New Delhi, 1975), pp. 332–334.

[7] There is one subtle way in which canonical and grand-canonical ensembles are *not equivalent even in equilibrium* precisely at first-order coexistence: In the canonical ensemble one obtains both coexisting phases *with an interface between them*; in the grand-canonical ensemble *only one or the other* phase appears (since the density is not fixed in this case, there is no need to pay for the extra interfacial free energy).

[8] H. Gould, and J. Tobochnik, *An Introduction to Computer Simulation Methods, Part 2* (Addison-Wesley, New York, 1988).

[9] J. Marro and J. L. Valles, J. Stat. Phys. **49**, 121 (1987); **49**, 89 (1987).

[10] R. J. Glauber, J. Math. Phys. **4**, 294 (1963).

[11] R. Bausch, H. K. Janssen, and H. Wagner, Z. Phys. B **24**, 113 (1976).

[12] P. C. Martin, E. D. Siggia, and H. A. Rose, Phys. Rev. A **8**, 423 (1973).