Phase Transitions in a Driven Lattice Gas with Repulsive Interactions

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We study a lattice gas with repulsive nearest-neighbor interactions driven to steady state by an external electric field E. Using Monte Carlo techniques on a two-dimensional system, we find, in the E-T plane, a line of second-order transitions joining a line of first-order ones, at a point which is probably tricritical. From a field theoretic model, we show that the operator associated with E is naively irrelevant for critical behavior. This expectation is borne out by the Monte Carlo result $\beta = \frac{1}{8}$.

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Phase transitions far from thermal equilibrium occur in a great variety of physical and biological systems. Because of the problems inherent in nonequilibrium statistical mechanics, it is of primary interest to formulate clearly the microscopic mechanisms governing the transitions. This is a prerequisite before more intricate analytic techniques (such as mean-field theories or renormalization-group approaches) can be tailored to seek a deeper understanding. Models adopted from equilibrium statistical mechanics have the advantage that their behavior is well understood, in terms of both a discrete lattice description and a coarse-grained continuum theory. If such a system is driven out of thermal equilibrium in a controlled way, its properties may be significantly modified.

Recently, a prototype model was proposed[1] for considering one specific type of nonequilibrium behavior, i.e., a system in steady state. It is the lattice gas with particle-conserving hopping dynamics under the influence of an external field E. The effect of E is analogous to that of an electric field on charged particles: It causes a bias of the hopping rates in a given direction $\hat{\mathbf{e}}$, induces a net current, and drives the systems away from equilibrium. One of the central issues is to determine if and how the Ising-type equilibrium phase transition is affected, when cooperative.

The driven lattice gas has attracted considerable attention.[1-10] With the focus almost entirely on models with short-ranged *attractive* ["ferromagnetic" (FM)] interactions, most results have been obtained following three major lines of approach: (i) direct Monte Carlo simulations in two[1-3] and three[4] dimensions; (ii) mean-field solutions, exact in the fast rate limit,[5,6] and (iii) renormalized field theoretic calculations of critical behavior.[7-9]

The essential observations from simulations are as follows: The phase-separation transition persists at all field strengths, with $T_c(E)$ an increasing function of E. At the critical density, it remains continuous, but the (measured) critical exponents are incompatible with their Ising values. In the treatment by van Beijeren and Schulman,[5] the hopping dynamics is simplified considerably, by assuming that longitudinal jumps (parallel to the field) occur much more frequently than transverse jumps. This "fast rate" limit allows for a separation of time scales in the master equation, effectively reducing the spatial dimension of the problem by one. Now the steady-state probability distribution can be obtained analytically, with mean-field exponents as one of the main results. These predictions are in agreement with field theoretic calculations, using renormalization group in an expansion about the upper critical dimension $d_c = 5$. Here, the main conclusions are the following: (a) The dynamics of the system cannot be formulated in terms of (the functional derivative of) a suitable Hamiltonian. (b) The jump rate at the fixed point is a fast rate limit. (c) The order-parameter exponent β, governed by a dangerous irrelevant operator, is $\frac{1}{2}$, to all orders in perturbation theory and for all $d > 2$.

In this Letter, we report Monte Carlo simulations, supported by analytical arguments, of the driven lattice gas with *repulsive* short-ranged ("antiferromagnetic") interactions. So far, the only known[1] properties are that E lowers the transition temperature so that the system is always disordered when driven by sufficiently strong fields. We studied, in some detail, the phase diagram in a corner of the (E,T) plane, where E and T are both of the order of T_N, the Néel temperature. (In our units, both Boltzmann's constant and the lattice spacing are 1.) We found a line of second-order transitions, starting at $(0,T_N)$, and a line of first-order ones, emerging from the $T=0$ axis. We believe that these lines join at a (nonequilibrium) tricritical point. We propose a field theoretic model, and have found that E is (naively) irrelevant for both critical and tricritical properties, for all $d > 2$. Our conjecture is that E remains so in $d=2$. Subsequent simulations support this conjecture, in the sense that our data are fitted by $\beta = \frac{1}{8}$ and $\nu = 1$ quite well. The rest of this Letter is devoted to a brief description of our simulation methods, data analysis, and the field theoretic mod-

el.

In an Ising lattice gas, a site i of the ($L\times L$ square) lattice may be occupied by a particle or empty. Using the labels $n_i=1$ and 0, respectively, the repulsive short-ranged interactions are modeled by the Hamiltonian $J\sum n_i n_j$, with $J>0$ and the sum over nearest-neighbor pairs. Employing standard Monte Carlo methods,[11] we simulate only $\rho\equiv\sum_i n_i/L^2=\frac{1}{2}$ systems. Evolving stochastically under Kawasaki[12] dynamics, the particles may only jump into a neighboring hole. The jump rates used are the usual Metropolis[11] ones, except when the particle jumps along (against) E, in which case they are enhanced (suppressed) by a factor $e^{E/T}$ ($e^{-E/T}$). With periodic boundary conditions imposed in both directions, the system has translational invariance, settling into a steady state eventually. In the absence of E, the system orders spontaneously for $T<T_N\approx 0.5673J$.[13] The particles preferentially occupy one of the two sublattices (say, white squares on a checkerboard). We naturally refer to this state as "antiferromagnetic" (AFM).

Our goal is to study the effects of the driving field E on this phase transition and to map out the phase diagram in the E-T plane. We performed simulations for E ranging from 0.5 to 2.5 (in units of J) and for T from 0.2 to 1.2 (in units of T_N). Runs are as long as 0.2×10^6 Monte Carlo steps per site (MCS).

The effects of E are much more subtle than for the FM case, since E is not directly coupled to the order parameter, the "staggered magnetization": $\phi_i\equiv(-1)^i\times(2n_i-1)$. Instead, E drives only the conserved density n_i. Using $\phi\equiv(1/L^2)\langle\sum_i\phi_i\rangle$ to identify phase transitions, we find that the critical temperature $T_c(E)$ decreases as E increases. Simulations at small E (0.5 and 0.75) show that the transition remains a second-order one. Contrary to the FM model, where strong spatial anisotropy is observed[3,4] even far from criticality, we find that anisotropy is mostly negligible and small even in the critical region. Thus, we invoke *isotropic* finite-size scaling[14] to explore the critical behavior, using high-precision data in systems with $E=0.5$ and $L=12$, 18, 24, 30, and 40. Following the suggestion by a field theoretic argument (see below) that E is *irrelevant* for this transition, we attempt to fit ϕ with an *equilibrium* scaling form with Onsager exponents: $\phi(L,T)=L^{\beta/\nu}X_{\pm}(\tau)$, where $\tau\equiv|1-T/T_c(E)|L^{1/\nu}$. Using $\beta=\frac{1}{8}$, $\nu=1$, and adjusting T_c in a plot of $\ln(\phi L^{-\beta/\nu})$ vs $\ln(\tau)$, all data points collapse onto one curve, X_+ (for $T>T_c$), or another, X_- (for $T<T_c$). Our result is $T_c=0.81\pm 0.01$ for $E=0.5$. For both large and small τ, $X_{\pm}$ has the well known[15] critical behavior of the order parameter in a finite system. Thus, we conclude that E is indeed irrelevant for critical properties of our system. This is believed to hold along the entire line of second-order transitions.

The transition continues to be of second order until $E\approx 1$, where hysteresis appears, becoming more pronounced as E is increased. For the present length of runs, hysteresis for $E\geq 1.5$ is so strong that the low-temperature branch is never reached by lowering T. On the other hand, ϕ decays rapidly from the low-T branch to the high-T one, when T is raised from $T=0$ beyond a certain temperature, which we denote by $T_u(E)$. Similarly, when we fix T and scan along E, we observe jumps between the two branches in both directions. This behavior, supported by studies of the distribution function of ϕ, signals a *first-order* transition. $T_u(E)$ represents an upper bound of the transition temperature, decreasing with larger E. We believe that this line of first-order transitions joins the second-order line at a tricritical point. Our data put it roughly at $E\approx 1$ and $T\approx 0.5$. More simulations are necessary to check this conjecture, determining more precisely the location and nature of this dynamically generated multicritical point.

If the field is increased further than a critical E_c, then AFM order is destroyed for any T, in contrast to the driven attractive case. This occurs when E is strong enough to overcome the repulsive force. Using a $T=0$ argument, one would naively expect E_c to be 3, since a particle will jump into a hole with three neighbors present. Upon closer examination, however, $E_c=3$ turns out to hold only for a system at $T\equiv 0$ and $\rho\equiv\frac{1}{2}$. For generic systems, E_c is just 2, since a local thermal excitation or defect reduces the number of particles around a hole to 2. For $E\geq 2$, an avalanche follows any initial jump, destroying AFM order.[16] Confirmed by simulations, this process takes only a short time ($\sim$400 MCS for $L=40$). We emphasize that this will occur when the system deviates from exactly half filled by a *single* particle, regardless of L. So, $\rho\equiv\frac{1}{2}$ stands for more than just $\rho=\frac{1}{2}$ (in the thermodynamic limit).

We summarize our findings in a phase diagram (Fig. 1). Note that the heavy line at $T=0$ and $2\leq E<3$ rep-

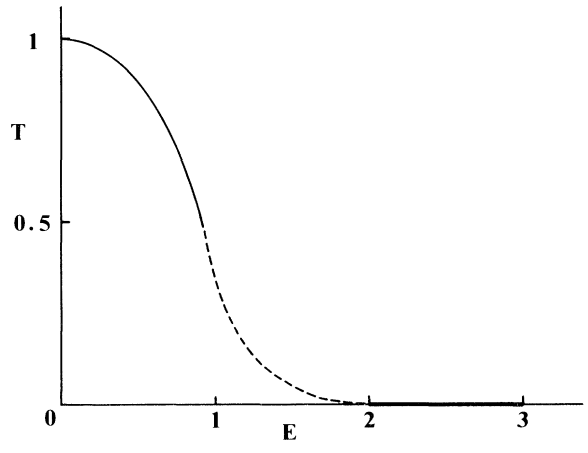

FIG. 1. Phase diagram in E-T plane. The unit for E/T is J/T_N. The solid (dashed) line represents second- (first-) order phase transitions. See text for an explanation of the heavy solid line.

resents an ordered state only if a $\rho \equiv \frac{1}{2}$ system is initially ordered. It is possible for a $\rho \equiv \frac{1}{2}$ finite system to evolve from disorder to compete order in a finite time. Whether this is *always* possible or whether glasslike minima exist is an intriguing, if merely theoretical, question. Finally, we remark that a $\rho \neq \frac{1}{2}$ system corresponds to an AFM model under a uniform magnetic field. For $E=0$, the Néel transition still exists, though at a different temperature. We believe that when such a system is driven, the lines of phase transitions will extend into sheets in E-T-ρ space.

Next we study the critical behavior by field theoretic techniques. There are two main ingredients in a continuum model: The ordering field "staggered magnetization," $\phi(x,t)$, and the "magnetization," $m(x,t)$, which is the coarse-grained $n_i - \frac{1}{2}$. Though nonordering and zero on the average, the latter is essential since E has an effect on the phase transition only via m. Taking into account the symmetries in ϕ and m, we first write a Landau-Ginzburg-Wilson Hamiltonian suitable for the critical dynamics[17] of an AFM with $E=0$:

$$H = \int d^d x [\tfrac{1}{2}(\nabla\phi)^2 + \tfrac{1}{2}\tau\phi^2 + g\phi^4/4! + \tfrac{1}{2}m^2 + \tfrac{1}{4}um^2\phi^2 + \cdots].$$

Of all the parameters, only τ depends on T essentially, vanishing at T_N (after renormalization). The effect of E is introduced, in the same way as for the FM case, by modifying the $E=0$ equation of motion for the particle density (m, in our case). Thus, the Langevin equations are

$$\frac{\partial\phi}{\partial t} = -\Gamma\frac{\delta H}{\delta\phi} + \xi, \quad \frac{\partial m}{\partial t} = \Lambda\nabla^2\frac{\delta H}{\delta m} - \Lambda(\mathbf{E}\cdot\nabla)m^2 + \zeta, \tag{1}$$

where Γ and Λ are Onsager coefficients, while ξ and ζ are Gaussian correlated noise terms. Note that E here is related to the E above by a complex but unessential way, just as H may be traced to $J\sum nn$.

Following the standard renormalization-group approach, we would ask if E is relevant to the Wilson-Fisher fixed point[18] g^*, which controls nonclassical critical behavior of the $E=0$ system. Before this question can be fully answered, we must compute d_E, the naive dimension of E. Casting (1) in a dynamic functional formalism,[19] we find $d_E = (2-d)/2$, in contrast to $(5-d)/2$ for the FM case.[7-9] Thus, for $d > 2$, the *Gaussian* fixed point is stable. We conjecture that g^* is also stable down to $d=2$. If the correction beyond d_E (in a $4-d$ expansion) is negative, then we can assert that Onsager exponents should be observed in our simulations along the entire line $T_c(E)$. Such a calculation is not entirely trivial, since u, which mediates the effects of g^* on E, is also naively irrelevant for $d > 2$.

Apart from fixed-point analysis, we could also examine the flow in J space under renormalization. Not surprisingly, all (transport) coefficients of gradient terms become anisotropic. Unlike the FM case, m does not order and ϕ is not diffusive so that anisotropy is not a dominant feature in criticality. To lowest order (E^2), the critical parameter τ is modified by a positive term, indicating a lowering of the transition temperature from T_N. On the other hand, g is shifted by a *negative* contribution, suggesting that $g(E^2)$ may vanish, as well as τ for a sufficiently large E. That would be the signal of a tricritical point, supporting our belief gleaned from simulation data. Using naive dimensional arguments again, one might predict that E is also irrelevant for tricritical behavior in $d \geq 2$. Since there is no such point in a $E=0$ system, more careful analysis is necessary before a clear picture of this *dynamically* generated tricritical system will emerge.

In conclusion, we studied a lattice gas with repulsive nearest-neighbor interactions driven to steady state by an external field E using two methods: Simulations on a discrete $d=2$ system and field theoretic analysis of a continuum model in any d. A phase diagram of the former is found, showing a line of second-order transitions joining a line of first-order ones, at a point which is probably tricritical. A finite-size scaling plot of a certain $E \neq 0$ critical system favors Onsager exponents. From a field theoretic analysis, we see more clearly the features that distinguish this system from the FM one. In the latter, the external field couples directly to the conserved ordering density and is naively relevant for $d < 5$, generating anisotropic critical parameters and necessitating an anisotropic dimensional analysis. In our case, E couples indirectly through an auxiliary, nonordering field. Naively irrelevant (for $d > 2$) and generating only trivial anisotropies, small fields do not affect critical behavior. On the other hand, large fields do create a rich and different system for interesting future investigations.

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[1]S. Katz, J. L. Lebowitz, and H. Spohn, Phys. Rev. B **28**, 1655 (1983); J. Stat. Phys. **34**, 497 (1984).

[2]J. L. Vallés and J. Marro, J. Stat. Phys. **43**, 441 (1986); **49**, 89 (1987); J. Marro and J. L. Vallés, J. Stat. Phys. **49**, 121 (1987).

[3]M. Q. Zhang, J.-S. Wang, J. L. Lebowitz, and J. L. Vallés, J. Stat. Phys. **52**, 1461 (1988).

[4]J. Marro, J. L. Lebowitz, H. Spohn, and M. H. Kalos, J. Stat. Phys. **38**, 725 (1985).

[5]H. van Beijeren and L. S. Schulman, Phys. Rev. Lett. **53**, 806 (1984).

[6]H. van Beijeren, R. Kutner, and H. Spohn, Phys. Rev. Lett. **54**, 2026 (1985); J. Krug, J. L. Lebowitz, H. Spohn, and M. Q. Zhang, J. Stat. Phys. **44**, 535 (1986).

[7]H. K. Janssen and B. Schmittmann, Z. Phys. B **64**, 503 (1986).

[8]K.-t. Leung and J. L. Cardy, J. Stat. Phys. **44**, 567 (1986).

[9]K. Gawadzki and A. Kupiainen, Nucl. Phys. **B269**, 45 (1986).

[10]K.-t. Leung, J. Stat. Phys. **50**, 405 (1988); A. Hernandez-Machado and D. Jasnow, Phys. Rev. A **37**, 626 (1988); K.-t. Leung, K. K. Mon, J. L. Vallés, and R. K. P. Zia, Phys. Rev. Lett. **61**, 1744 (1988); Phys. Rev. B (to be published); J. L. Vallés, K.-t. Leung, and R. K. P. Zia, J. Stat. Phys. (to be published).

[11]For reviews, see K. Binder, in *Applications of Monte Carlo Methods in Statistical Physics,* edited by K. Binder (Springer-Verlag, Berlin, 1984).

[12]K. Kawasaki, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1972), Vol. 2.

[13]L. Onsager, Phys. Rev. **65**, 117 (1944).

[14]M. E. Fisher, in *Critical Phenomena,* International School of Physics "Enrico Fermi," Course 51, edited by M. S. Green (Academic, New York, 1971).

[15]D. P. Landau, Phys. Rev. B **13**, 2997 (1976).

[16]This observation was made by H. van Beijeren (private communication).

[17]B. I. Halperin, P. C. Hohenberg, and S.-k. Ma, Phys. Rev. B **10**, 139 (1974). For a review, see P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).

[18]K. G. Wilson and M. E. Fisher, Phys. Rev. Lett. **28**, 240 (1972). For a review, see K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).

[19]H. K. Janssen, Z. Phys. B **23**, 377 (1976); R. Bausch, H. K. Janssen, and H. Wagner, Z. Phys. B **24**, 113 (1976); C. De-Dominicis, J. Phys. (Paris), Colloq. **37**, C1-247 (1976); H. K. Janssen, in *Dynamic Critical Phenomena and Related Topics,* edited by Ch. Enz (Springer-Verlag, Berlin, 1979), p. 25.