Critical Behavior of the Pair Contact Process

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I study a nonequilibrium lattice model, the *pair* contact process, in which pairs of particles annihilate with probability p or else create a particle at a vacant nearest neighbor. The model exhibits a continuous phase transition from an active state, with an ongoing production of particles, to an absorbing state without pairs. The model has infinitely many absorbing states. Computer simulations in 1D yielded critical exponents consistent with directed percolation, for the first time placing a model with infinitely many absorbing states firmly in the directed-percolation universality class.

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The study of nonequilibrium many-particle systems is an important problem in many branches of physics, chemistry, biology, and even sociology [1,2]. Much attention has been given to nonequilibrium models exhibiting a continuous phase transition from an active steady state to a *unique* absorbing state (a state in which the system is trapped). One of the major achievements in the study of nonequilibrium phase transitions is the discovery that a wide variety of models exhibiting this kind of transition belong to the same universality class. Among these models the best known are probably the contact process [3–5], Schlögl's first and second models [6–8], directed percolation (DP) [9–12], Reggeon field theory (RFT) [13–16], and the ZGB (Ziff-Gulari-Barshad) model [17–19]. The study of these and many other models [20–26] demonstrates the robustness of DP critical behavior in spite of quite dramatic differences in the evolution rules of the various models. Presently there is thus substantial evidence in favor of the hypothesis that models with a scalar order parameter exhibiting a continuous transition to a *unique* absorbing state generically belong to the universality class of directed percolation. This *DP conjecture* was first put forward by Grassberger [8] and Janssen [7] and later extended by Grinstein, Lai, and Browne [18] to multicomponent models such as the ZGB model.

Whereas the universality of DP critical behavior for models with a single absorbing state seems well established, the study of models with more than one absorbing state is still in its very beginning. That models with more than one absorbing state can exhibit new critical behavior was first demonstrated by Grassberger, Krause, and von der Twer [27] in a study of a model involving the processes $X \rightarrow 3X$ and $2X \rightarrow 0$. This model is very similar to a class of models known as branching annihilating walks (BAW's) [24]. In the BAW a particle jumps, with probability p, to a nearest neighbor and if this site is occupied both particles annihilate. With probability $1-p$ the particle produces n offspring which are placed on the neighboring sites. If an offspring is created on a site which is already occupied, it annihilates with the occupying particle leaving an empty site. For n even these models have non-DP behavior [25] whereas the behavior for n odd is compatible with DP [26]. Note that in both the model proposed by Grassberger, Krause, and von der Twer and in BAW's with an even number of offsprings the number of particles is conserved modulo 2. This conservation law might be responsible for the non-DP behavior.

Models with infinitely many absorbing states [28] arise naturally in the study of reactions catalyzed by a surface as soon as the absorption mechanism for the various species requires more than one vacant site. Two such models, the dimer-dimer model [29] and the dimer-trimer model [30], were introduced recently.

The dimer-dimer (DD) model is a model for the oxidation of hydrogen on a metal surface. O_2 adsorption is attempted with probability p and H_2 adsorption with probability $1-p$. Both O_2 and H_2 require a nearest neighbor pair of vacancies and dissociate upon adsorption. Nearest neighbor H and O react to form OH residing on a single site, OH reacts with H (OH) forming H_2O (leaving behind one O) which desorbs immediately. In addition, H is allowed to diffuse. When $p < p_1$, the steady state is an absorbing state with a mixture of adsorbed O and OH and isolated single vacancies (clearly there are infinitely many such states). When $p > p_2$ the lattice becomes completely covered with H, which is thus a unique absorbing state. For $p_1 < p < p_2$ there is an active steady state with an ongoing production of H_2O. In the vicinity of p_1 one has $\rho_H \propto (p-p_1)^{\beta_H}$ and $\rho_{O+OH}^{sat} - \rho_O - \rho_{OH} \propto (p-p_1)^{\beta_O}$, where $\rho_{O+OH}^{sat} \simeq 0.907$ is the saturation value of O and OH coverage. Albano [29] estimates that $\beta_H = \beta_O \sim \frac{1}{2}$ with an uncertainty of (5–10)%. These results may be seen as an indication of a new universality class though the results could be marginally consistent with DP behavior, $\beta \simeq 0.586 \pm 0.014$ [10,14] for directed percolation in $(2+1)$ dimensions.

In the dimer-trimer model dimers A_2 may adsorb onto a nearest neighbor pair of vacancies and subsequently dissociate. Likewise a trimer B_3 may undergo dissociative adsorption onto three nearest neighbor vacancies. A and B nearest neighbors react instantly and the product AB desorbs. A_2 adsorption is attempted with probability p and B_3 adsorption with probability $1-p$. Computer

simulations [30] on triangular lattices showed a trimer saturated state for $p < p_1$, a dimer saturated state for $p > p_2$, and an active steady state for intermediate values. A saturated state is a configuration with only isolated empty sites left. Such states are absorbing and there are infinitely many of them. The transition at $p_1 = 0.3403(2)$ is continuous whereas the transition at $p_2 = 0.4610(8)$ is discontinuous. Critical exponents β_A and β_B may be defined as $\rho_A \propto (p - p_1)^{\beta_A}$ and $\rho_B^{\rm sat} - \rho_B \propto (p - p_1)^{\beta_B}$, where $\rho_B^{\rm sat}$ is the saturation concentration of B at p_1. Steady-state computer simulations [30] yielded $\beta_A = 0.80(6)$ and $\beta_B = 0.63(5)$. The estimate for β_B is consistent with DP behavior whereas the estimate for β_A is well above the DP value. Note, however, that one expects $\beta_A = \beta_B$ on general grounds (there is no reason to suspect two critical fields [18]). Given that the A concentration is very low close to p_1 I am inclined to trust the estimate for β_B over the estimate for β_A.

While the results for the dimer-dimer and dimer-trimer models suggest that models with infinitely many absorbing states may exhibit non-DP behavior, the accuracy of the estimates for β is not so good as to definitely rule out DP behavior. In this Letter I study a simple one-dimensional model, which I call the *pair* contact process (PCP). I have chosen to study this model because it is one of the simplest models with infinitely many absorbing states exhibiting a continuous phase transition. In the PCP nearest neighbor particle pairs annihilate with probability p or else create a new particle at a randomly chosen nearest neighbor provided it is vacant. Any state without pairs is absorbing. Note that the number of such states $> 2^{N/2}$, where N is the number of lattice sites. Any finite system will eventually become trapped in such a state. In addition to this trivial state the system has (in the infinite-size limit) a nontrivial ("active") steady state, with a nonzero average concentration ρ of pairs, when p is sufficiently small. The region of the phase diagram in which there is an active steady state is called the supercritical region, as opposed to the subcritical region in which the absorbing state is the only steady state. The PCP exhibits a continuous phase transition from the active to the absorbing state at a critical value p_c. I will assume that the concentration of pairs is the appropriate order parameter. The absorbing states are the ones without pairs, so in a sense there is a unique absorbing state from the pair point of view. The presence of infinitely many absorbing states on the particle level is, however, a new feature which could lead to a new critical behavior. Note also that the absorbing states of the dimer-dimer and dimer-trimer models are the states without any pairs of empty sites.

We assume that the critical behavior of quantities such as the order parameter $\bar{\rho}$ (where the overbar indicates the steady-state value) have power-law dependence close to the critical point:

$$\bar{\rho} \propto |p_c - p|^{\beta}, \tag{1}$$

where β is the order parameter critical exponent. Note that Eq. (1) holds true only in the limit of infinite system size. As in equilibrium second-order phase transitions we assume that the nonequilibrium system features a length scale which diverges at criticality as

$$\xi(p) \propto |p_c - p|^{-\nu_\perp}, \tag{2}$$

where $\nu_\perp$ is the correlation length exponent in the space direction. Any measurable quantity will depend strongly on system size once the correlation length becomes comparable to the linear extension L of the system. Steady-state simulations are also complicated by a diverging relaxation time near the critical point. Consequently, in order to obtain reliable results close to a critical point one has to study large systems over long times. In the absence of an independent estimate p_c becomes a fitting parameter (as are the critical exponents), and thus a possible source of error.

Steady-state computer simulations may be greatly enhanced by finite-size scaling analysis. The idea of finite-size scaling was pioneered by Fisher and co-workers in the early 1970's [31,32]. Here I will follow the work of Aukrust, Browne, and Webman [21] and show how finite-size scaling can be used in the study of nonequilibrium phase transitions. Another very efficient method for studying the critical behavior of models with absorbing states was pioneered by Grassberger and de la Torre [16] and has since been used extensively [8,12,19,20, 22,23,26].

From the nature of the model it is clear that small systems will enter the absorbing state fairly quickly, even when $p < p_c$. In Fig. 1 I show the concentration of pairs as a function of time at $p = 0.0771$ with $L = 128$. Each time step equals on the average one attempted update per lattice site and throughout I used periodic boundary conditions. $\rho(t)$ almost immediately reaches a reasonably steady value somewhat obscured by large fluctuations. After the system has reached this quasisteady state it can spend a long time there before it finally enters the absorb-

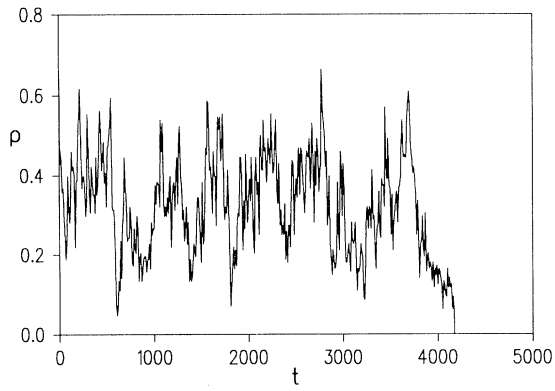

FIG. 1. Typical time evolution of the concentration of pairs for $L = 128$ at $p = 0.0771$.

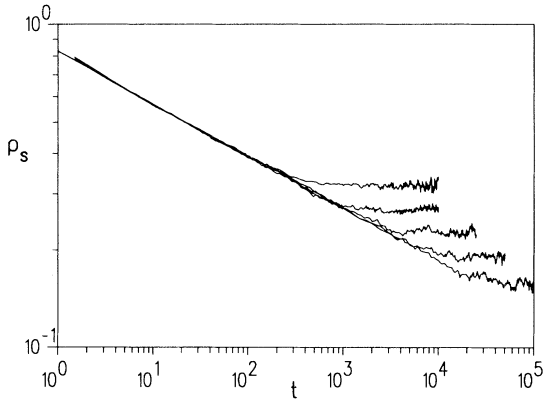

FIG. 2. Average number of pairs in the surviving samples, $\rho_s(p,L,t)$, as a function of time at $p=0.0771$ for, from top to bottom, $L=128$, 256, 512, 1024, and 2048.

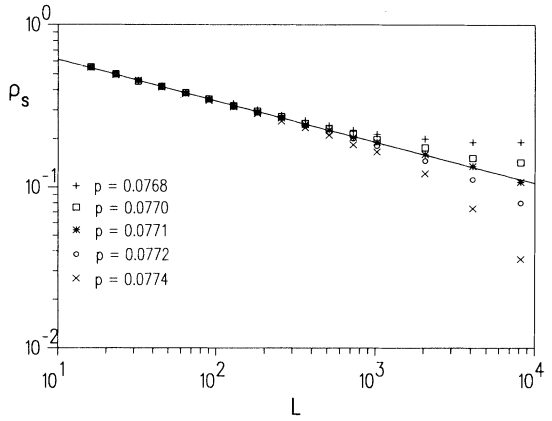

FIG. 3. Log-log plot of $\rho_s(p,L)$ vs L. The slope of the line is $\beta/\nu_\perp=0.255$.

ing state. Figure 2 shows $\rho_s(p,L,t)=\langle\rho(p,L,t,s)\rangle$ vs t for various values of L at $p=0.0771$. $\rho(p,L,t,s)$ is the coverage fraction for a particular sample s. The subscript s indicates an average of only those samples which have not yet entered the absorbing state. The number of initial samples varied from 2000 for $L=128$ to 250 for $L=2048$; in all cases at least 200 samples survived to the end of the simulations. Figures 1 and 2 show that in spite of a strong tendency to enter the absorbing state ρ_s does attain a well-defined value and we can thus study $\rho_s(p,L)$ as a function of p and L in the critical region.

The ansatz underlying finite-size scaling is that the various quantities depend on system size through the variable $|p_c-p|L^{1/\nu_\perp}$. Thus we assume that the order parameter depends on system size and distance from the critical point as

$$\rho_s(p,L)\propto L^{-\beta/\nu_\perp}f((p-p_c)L^{1/\nu_\perp}), \tag{3}$$

such that at p_c

$$\rho_s(p_c,L)\propto L^{-\beta/\nu_\perp} \tag{4}$$

and

$$f(x)\propto x^\beta \text{ for } x\to\infty, \tag{5}$$

so that Eq. (1) is recovered when $L\to\infty$ in the critical region. For values of p in the supercritical regime ρ_s should be independent of L, for $L\gg\xi(p)$. In the subcritical regime one expects ρ_s to decay faster than a power law. Thus p_c may be determined as the value of p yielding a straight line in a log-log plot of ρ_s vs L. Figure 3 shows $\rho_s(p,L)$ as a function of L on a log-log scale for various values of p in the critical region. The results for $\rho_s(p,L)$ were obtained by performing a time average of $\rho_s(p,L,t)$ in the quasisteady state. The number of time steps t and independent samples N varied from $t=1000$, $N=25000$ for $L=16$ to $t=500000$, $N=100$ for $L=8192$. From this we clearly see that $p=0.0771$ is consistent with a power-law behavior, whereas $p=0.0770$ is supercritical and $p=0.0772$ is subcritical, leading to the estimate $p_c=0.0771(1)$, where the figure in parenthesis is the estimated uncertainty. From the slope of the critical curve I estimate that $\beta/\nu_\perp=0.255(5)$. This value is in excellent agreement with that obtained from directed-percolation-type models $\beta/\nu_\perp=0.2524(5)$ using the values $\beta=0.2769(2)$ [33] and $\nu_\perp=1.0972(6)$ [34].

Once a precise estimate for p_c has been obtained an analysis of the data for $\bar{\rho}$ may yield a fairly accurate estimate for β. Figure 4 is a log-log plot of $\bar{\rho}$ versus the distance from the critical point, p_c-p, with $p_c=0.0771$. The results for $\bar{\rho}$ were obtained by averaging over 100 independent samples. The number of time steps and system sizes varied from $t=5000$, $L=512$ far from p_c to $t=500000$, $L=8192$ closest to p_c. From these results I estimate $\beta=0.28(1)$, which again is in excellent agreement with the value for directed percolation.

From Fig. 2 we see that the initial decay of ρ_s, before

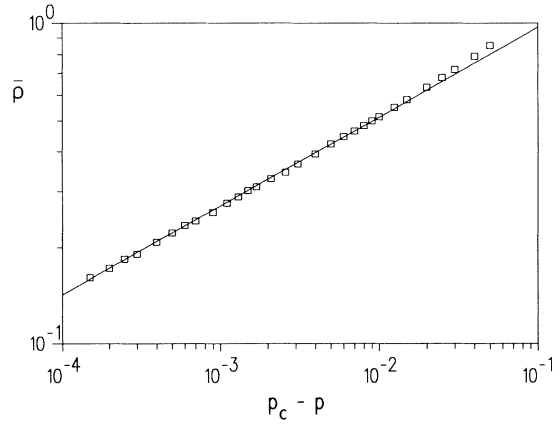

FIG. 4. Log-log plot of the steady state concentration of pairs $\bar{\rho}$ vs p_c-p with $p_c=0.0771$. The slope of the line is $\beta=0.277$.

entering the quasisteady state, follows a power law. Scaling arguments [21] show that the exponent θ characterizing this decay is given by the relation $\theta=\beta/\nu_{\|}$, where $\nu_{\|}$ is the correlation length exponent in the time direction. From the results of Fig. 2 I estimate $\theta=0.160(5)$. This is in excellent agreement with directed percolation, for which the estimate $\nu_{\|}=1.733(1)$ [34] yields $\theta=9.1598(3)$.

The results for the critical exponents of the PCP strongly suggest that the model belongs to the DP universality class. With pairs as the fundamental entity the PCP may be seen as having a unique absorbing state, namely the state without pairs. Likewise one may argue that the dimer-dimer and dimer-trimer models has just one absorbing state, e.g., the state with no pairs of empty sites. Though the exponent estimates are only marginally consistent with directed percolation it does not seem impossible that these models also belong to the DP universality class. It thus seems possible that the DP conjecture may be extended even to models with infinitely many absorbing states, at least as long as the absorbing states can be characterized by the vanishing of a single quantity, e.g., the concentration of pairs in the PCP. The non-DP behavior of the model proposed by Grassberger, Krause, and von der Twer [27] and BAW's with an even number of offsprings [25] might be contributed to the additional conservation law (particle number conserved modulo 2) not present in other models.

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