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First-order phase transition in a one-dimensional nonequilibrium model

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We present an example of a single-component, one-dimensional interacting particle system with a discontinuous transition into an absorbing state. The basic processes in the model are spontaneous annihilation ($X \rightarrow 0$), autocatalytic creation by trimers ($3X \rightarrow 4X$), and hopping. The transition is continuous, and in the directed percolation class, for low diffusion rates, and *first order* for sufficiently high diffusion rates. The transition in a similar model with creation by pairs ($2X \rightarrow 3X$) remains continuous even at high diffusion rates.

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I. INTRODUCTION

Nonequilibrium phase transitions continue to attract great interest in physical and biological sciences [1,2]. Theoretical efforts have focused on simple lattice models or interacting particle systems [3] which describe nonequilibrium transitions in ionic conductors [4,5], surface catalysis [6], and autocatalytic chemical systems [7]. Many of these models exhibit a transition into an absorbing vacuum state. Typically the transition is continuous and belongs to the universality class of directed percolation [8,9]. Here we present an example of a one-component, one-dimensional model with a discontinuous transition into an absorbing state.

Consider a population of "particles" residing on the sites of a lattice (with at most one particle per site), which evolves via spontaneous annihilation ($X \rightarrow 0$), autocatalytic creation [$nX \rightarrow (n+1)X, n \geq 1$], and nearest-neighbor hopping. The simplest example ($n=1$) is the *contact process* (CP) [10] in which particles disappear at rate 1 and create new particles at a (vacant) nearest-neighbor site, at rate λ. The steady-state density $\bar{\rho}$ grows continuously from zero as λ is increased beyond a critical value λ_c [3,11]. The CP is a particularly simple realization of the universality class encompassing directed percolation and Reggeon field theory [3,12,13]; the same critical behavior is found in models describing diverse nonequilibrium processes [14–21]. The variety of models exhibiting directed percolation transitions lends strong support to the proposal [14] that such critical behavior is *generic* for continuous transitions into a unique absorbing state.

A question naturally arises, in attempting to comprehend the range of nonequilibrium phase transitions: Under what conditions will a system exhibit a *discontinuous* transition into an absorbing state? This issue arose in the context of autocatalytic chemical models [1,7,22]. Schlögl's first model is equivalent to a mean-field or rate equation description of the CP, while his *second* model involves autocatalytic creation by pairs ($2X \rightarrow 3X$). In its original mean-field formulation, the latter exhibits a *first-order* transition, because (in mean-field theory), the particle production rate is proportional to ρ^2. Will a strictly local version of the model, with creation only by nearest-neighbor pairs (a *pair-creation* model, in our terminology), show a discontinuous transition? Simulations [14] showed that the transition is actually *continuous* in one and two space dimensions, and discontinuous when $d=4$. Thus $d=4$ marks the upper critical dimension, below which mean-field predictions are qualitatively incorrect. For $d<4$ the particles are strongly clustered so that the production rate is proportional to ρ not ρ^2.

The question posed above may be restated: What is the simplest model with short-range interactions that *does* exhibit a discontinuous transition into an absorbing state? We shall present a likely candidate. Our criteria for "simplicity" include a restriction to one space dimension and to a single species of particle. A number of two-component models—for example, the Ziff-Gulari-Barshad model [6]—show discontinuous transitions. The only *single-component* local model we know of, with a discontinuous transition for small d, is the stochastic cellular automaton devised by Bidaux, Boccara, and Chaté (BBC) [23]. The transition in the BBC model is first order for $d \geq 2$, but continuous (and in the directed percolation class [21]), in one dimension. The BCC process involves interactions of a site with eight neighbors, so it is not as simple as one might hope.

Before considering more complicated processes, we should try to rule out the possibility of a first-order transition in the pair-creation model. We therefore begin by examining the pair-creation model under rapid diffusion, which might be expected to show mean-field-like behavior. Our simulation results indicate that this is quite unlikely: the transition remains continuous even when 95% of all attempted moves are diffusive. Another direction is suggested by recent results on models with competing diffusion and multiparticle *annihilation* [19,20,24,25]. It turns out that a three-particle annihilation rule leads to a new (reentrant) phase diagram, not observed for one- or two-particle annihilation. Thus we are motivated to study the competition between diffusion and a multi-particle birth process in a *triplet*-creation model. This system is the simplest we have been able to devise, which exhibits a discontinuous transition. Definitions of the models are given in the following section. Section III presents our simulation results, followed in Sec. IV by a brief discussion of theoretical approaches.

II. MODELS

We consider interacting particle systems on a one-dimensional lattice. The configuration is conveniently described in terms of occupation variables σ_i, with $\sigma_i=1$ (0) for site i occupied (vacant). The triplet-creation model involves three elementary processes.

Creation: Site i is chosen at random. If $\sigma_{i-1}=\sigma_i=\sigma_{i+1}=1$, then one of the sites $i+2$ or $i-2$ is chosen at random and a new particle is placed at the chosen site, provided this site is empty (if this site is already occuppied no creation occurs).

Annihilation: Site i is chosen at random. If $\sigma_i=1$ it is set to zero.

Hopping: Site i is chosen at random and σ_i and σ_{i+1} are interchanged.

The system evolves via a random sequence of hopping, creation, and annihilation processes, which occur with probability D, $(1-D)\lambda/(1+\lambda)$, and $(1-D)/(1+\lambda)$, respectively. The *pair*-creation model evolves in the same manner, except that creation is contingent upon the occupancy of just two neighboring sites (i.e., i and $i+1$). We are interested in the steady-state and time-dependent properties of these models, as functions of the diffusion rate D and the creation rate λ.

III. SIMULATIONS

Steady-state properties of the pair- and triplet-creation models were estimated from Monte Carlo simulations on a lattice of 10 000 sites with periodic boundary conditions. A study at a particular D value began from a filled lattice, with λ set well above its critical value. In that regime relaxation times are quite short, but as λ approaches the phase boundary at λ_c density fluctuations become larger and longer lived. Typical run lengths were $(1-2)\times 10^5$ lattice updates (in which each site is chosen once, on average); close to the transition as many as 6×10^5 updates were employed. A block-averaging procedure was used to estimate uncertainties [26].

The results for the steady-state density $\bar{\rho}$ in the pair- and triplet-creation models are presented in Figs. 1 and 2, respectively. The density in the triplet-creation model exhibits a substantial discontinuity—clear evidence of a first-order transition—for $D>0.85$. No gap is seen in the pair-creation data, even for $D=0.95$. We have found, however, that it is nearly impossible to maintain steady states with density less than 0.1, so it is very difficult to distinguish a continuous from a weakly first-order transition on the basis of the steady-state density. To obtain a more complete picture we have examined time-dependent behavior and hysteresis.

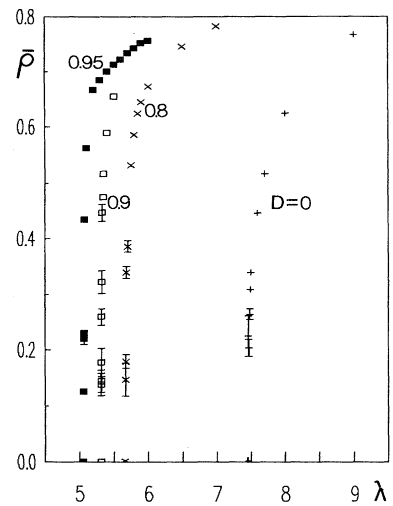

FIG. 1. Average density vs creation rate in steady-state simulations of the pair-creation model at hopping fractions $D=0$, 0.8, 0.9, and 0.95.

The time-dependent simulation method is based on the expectation—confirmed in numerous studies [14,17,20,21]—of power laws governing the evolution at the critical point. One studies the evolution of the system over a large number independent runs, always starting from a configuration very near to the absorbing state. [For each (λ, D) value studied, we performed between 10^4 and 5×10^5 runs, starting from a cluster of two (three) particles in the pair- (triplet-) creation model, in an otherwise vacant lattice.] Each run continues as long as particles remain in the system, up to a fixed maximum time t_M. The lattice is sufficiently large that no particles reach the boundary during a run. We follow the evolution of n_t, the mean particle number at time t, and of the sur-

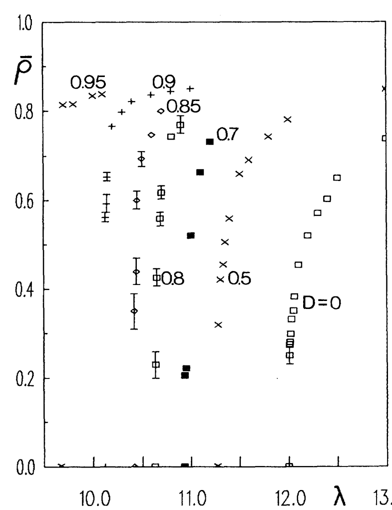

FIG. 2. Average density vs creation rate in steady-state simulations of the triplet-creation model at hopping fractions $D=0$, 0.5, 0.7, 0.8, 0.85, 0.9, and 0.95.

vival probability P_t. At a critical point, these quantities follow asymptotic power laws [27,28]:

$$n_t \approx t^{\eta} , \tag{1}$$

$$P_t \approx t^{-\delta} . \tag{2}$$

For directed percolation in 1+1 dimensions, the exponents take the values [12] $\delta = 0.162(4)$ and $\eta = 0.317(2)$, where the numbers in parentheses indicate the uncertainty in the last figure. The subcritical regime is characterized by exponential decay; for $\lambda > \lambda_c$ one observes linear growth in n_t and a nonzero limiting value for P_t. Power laws are not expected at a first-order transition: since correlations are of finite range, P_t and n_t should decay exponentially. Thus asymptotic power-law behavior of the survival probability and particle number indicate a continuous transition. Conversely, the absence of power-law scaling (i.e., in a range of λ values including the transition point) implies that the transition is first order.

Time-dependent simulations at a particular value of D covered a narrow range of λ values, including the estimate for the transition from the steady-state simulations. An independent estimate of critical value $\lambda_c(D)$ was obtained by the condition that logarithmic plots of P_t and n_t be asymptotically straight. Examples of power-law evolution are shown in Figs. 3 and 4 for the pair and triplet models, respectively. In all cases where power-law evolution was observed, the steady-state and time-dependent estimates for λ_c were in close agreement. Estimates for the critical exponents η and δ can be obtained from logarithmic plots of n_t and P_t. Greater precision is afforded by an analysis of the local slopes of such plots [28]; this method was applied to the triplet-creation model simulations. If power-law evolution is not observed at any λ value near the (steady-state) transition value (i.e., P_t and n_t decay exponentially), we conclude that the transition is first order. In this case the transition found in the steady-state simulations actually marks a spinodal.

We find that the transition in the pair-creation model remains continuous (and in the directed percolation class) for $D \leq 0.95$, confirming the conclusions drawn from the steady-state simulations. The transition in the triplet-creation model is continuous for $D < 0.8$, but it is clearly first order for $D \geq 0.9$. For $D = 0.9$, the active steady state persists for $\lambda \geq \lambda_c = 10.13$, but there is no evidence of power-law behavior in P_t or n_t at this point. In fact, n_t decreases monotonically, even at very long times ($t_M = 50\,000$), for $\lambda < 10.3$. Thus the time-dependent simulation results confirm that the triplet-creation model exhibits a tricritical point at $\lambda = \lambda_t \simeq 10.42$, $D = D_t \simeq 0.85$. For $D > D_t$ the simulations yield phase stability boundaries ("spinodal" lines) λ_- and λ_+. For $\lambda < \lambda_+$ the vacuum is locally stable while the active state remains locally stable for $\lambda > \lambda_-$. We determined $\lambda_+(D)$ in time-dependent simulations, using the criterion that the long-time ($t = 5 \times 10^4$) survival probability be nonzero but very small ($P_t \simeq 10^{-5}$). The phase diagram of the triplet-creation model is displayed in Fig. 5, which also shows a mean-field theory prediction to be discussed below.

Our results for phase boundaries and critical exponents are summarized in Table I. The exponents measured at continuous transitions are all consistent with directed percolation values, but there is some suggestion of a crossover to new values for $D = 0.95$ in the pair-creation model and for $D = 0.8$ in the triplet model. In the absence of diffusion (Fig. 4, open symbols), the approach to power-law evolution is quite rapid. In the presence of diffusion (Fig. 3, solid symbols in Fig. 4) the asymptotic regime is preceded by a transient period of exponential decay, whose duration increases with increasing D.

A key aspect of discontinuous phase transitions is hys-

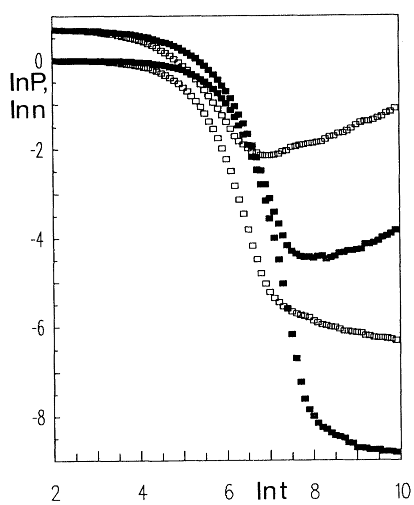

FIG. 3. Survival probability P_t and average particle number n_t in time-dependent simulations of the pair-creation model. Open symbols: $D = 0.9$, $\lambda = 5.35$; solid symbols: $D = 0.95$, $\lambda = 5.15$. The upper curve in each pair represents n_t, the lower one, P_t.

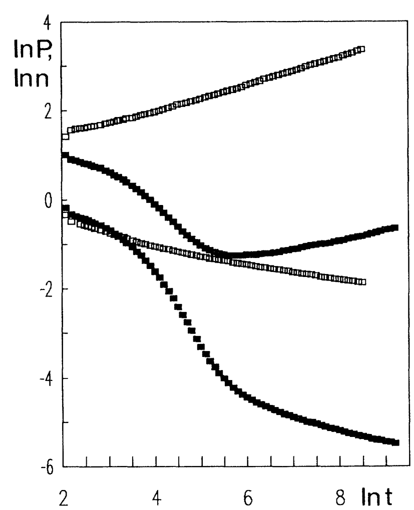

FIG. 4. Survival probability and average particle number as in Fig. 3, but for the triplet-creation model. Open symbols: $D = 0$, $\lambda = 12.0$; solid symbols: $D = 0.7$, $\lambda = 10.93$.

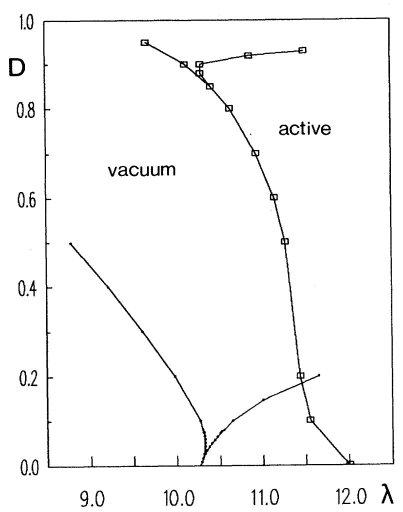

FIG. 5. Phase diagram for the triplet-creation model. The squares represent simulation results, connected by lines as a guide. The solid lines are mean-field-theory predictions for the phase boundaries.

teresis: In a regime allowing multiple locally stable phases, the state of the system depends strongly upon its history. Of course, in the present case the vacuum state admits no escape, while the active state (in a finite system) is strictly speaking metastable, but with a lifetime much longer than the time scale of the simulations. To study hysteresis, we modify the model to include a small rate κ of *spontaneous* particle creation. (Bidaux, Boccara, and Chaté [23] employed this strategy to study hysteresis in the model they devised.) We expect that for κ sufficiently small, the active and vacuum phases of the original triplet-creation model become distinct high- and low-density phases. If the transition (in the absence of spontaneous creation) is discontinuous, then it is reasonable to expect that for small κ the system will exhibit hysteresis between distinct high- and low-density phases, as λ is varied (with D and κ held constant). (If the transition in the original model were continuous, it would be destroyed by spontaneous creation.) We performed simulations of the triplet-creation model with $D=0.9$ and $\kappa=0.03$, on a lattice of 1000 sites (the smaller system size eliminates the need for very long relaxation times). The results, shown in Fig. 6, clearly demonstrate hysteresis.

TABLE I. Phase boundaries and critical exponents for the pair- and triplet-creation models.

D	λ_c	δ	η
	pair	creation	model
0.9	5.35(1)	0.163(3)	0.35(3)
0.95	5.15(1)	≈ 0.1	≈ 0.4
	triplet	creation	model
0	12.00(1)	0.158(8)	0.312(10)
0.1	11.55(1)		
0.2	11.435(15)	0.164(6)	0.305(10)
0.5	11.27(1)		
0.6	11.15(1)	0.170(6)	0.32(2)
0.7	10.935(10)	0.17(1)	0.32(1)
0.8	10.64(1)	0.20(5)	0.25(5)
0.85	10.415(5)		
	λ_-	λ_+	
0.90	10.12(1)	10.30(2)	
0.95	9.67(1)	≈ 17	

Further study of the model with spontaneous creation is in progress. In particular it would be interesting to study the coexistence of the two phases, and the interface between them, but establishing a stable interface appears to be quite difficult. We expect that with increasing κ the distinction between the high- and low-density phases is diminished, and finally vanishes at a critical value $\kappa_c(D)$.

Additional insight into the phase behavior of the triplet-creation model is afforded by examining the spatial distribution of particles. To this end we divide the system into blocks of 100 sites, and follow the evolution of the block-averaged density. Figure 7 shows a typical sequence of profiles (at intervals of 10^4 lattice updates), in a system close to the phase boundary λ_- ($D=0.95$, $\lambda=9.66$). The profiles clearly show distinct vacuum and high-density regions corresponding to the two locally stable phases. Histograms of such block density profiles show a bimodal distribution, with a very narrow peak at $\rho=0$ and a broader one near $\rho=0.84$. The latter peak maintains a nearly constant position and shape while its height gradually decreases as $\lambda \searrow \lambda_-$. This is further evidence of a well-defined high-density phase coexisting with vacuum.

IV. DISCUSSION

At the level of a Landau-Ginzburg-type theory, one may describe the phase behavior of the CP and related

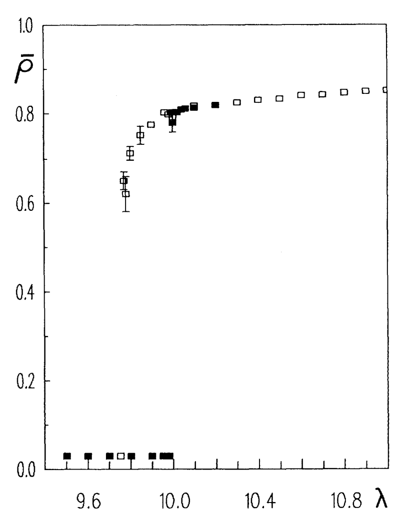

FIG. 6. Hysteresis loop observed in steady-state simulations of the triplet-creation model, with $D=0.9$ and spontaneous creation rate $\kappa=0.03$. Open symbols: gradually decreasing λ, starting at high density; solid symbols: gradually increasing λ, starting at low density.

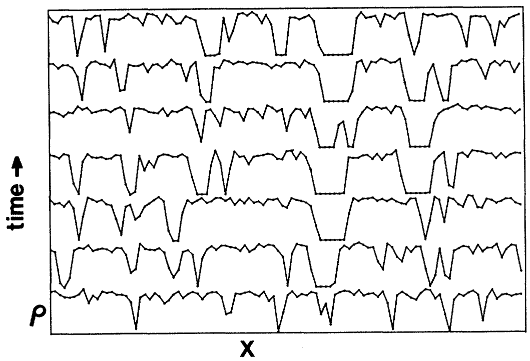

FIG. 7. Evolution of the block density profile in triplet-creation model with $\lambda=9.66$ and $D=0.95$. Each point represents the density of a 100-site block. Time increases toward the top of the plot; successive profiles are presented at intervals of 10^4 lattice updates.

models in terms of the evolution of a scalar order-parameter field:

$$\frac{\partial\rho(x,t)}{\partial t}=-a\rho(x,t)-b\rho(x,t)^2-c\rho(x,t)^3+D\nabla^2\rho(x,t) .$$

The uniform solution $\rho(x,t)=\bar{\rho}$ exhibits a critical point at $a=0$, for $b,c>0$, a first-order transition at $a=b^2/4c$, for $b<0$, $c>0$, and a tricritical point at $a=0$ for $b=0$, $c>0$. Janssen [29] showed that this sort of equation yields a qualitatively correct description of the critical point, when a Gaussian white-noise term that respects the absorbing state at $\rho=0$ is added. Ohtsuki and Keyes [30] applied this field-theoretic approach to calculate nonequilibrium tricritical exponents. However, Grassberger [14,31] has pointed out serious difficulties in the application of the field-theoretic formalism to models with multiparticle-creation rules. In particular it is not obvious how to identify the order parameter ρ; it appears more appropriate to associate it with the density of *clusters* than with the particle density. Another difficulty is that the parameters appearing in Eq. (3) represent effective, macroscopic rates; their dependence upon the microscopic rates λ and D is unknown. Thus, while the field-theoretic formalism may yield critical exponent values, it is not useful for predicting the phase diagrams of the models considered here.

A more straightforward method for predicting the phase diagram is provided by dynamic mean-field theory [32], in which one considers the evolution of densities of clusters of various sizes. An exact description would of course involve an infinite hierarchy of equations. A tractible, approximate theory is obtained by factorizing all probabilities for clusters of more than n sites, yielding a closed set of (nonlinear) equations for the evolution of the n-site cluster densities. We have studied the triplet-creation model in the four-site approximation (there are seven independent equations at this level). The resulting phase diagram is shown in Fig. 5: It is qualitatively correct in that it predicts a change from a continuous to a first-order transition. The location of the tricritical point (near $D=0.017$) is very far from the simulation result, however. (Mean-field theories employing smaller clusters predict a first-order transition independent of D.)

It is a commonplace that mean-field-like behavior obtains in the rapid diffusion limit. (Such limiting behavior has been rigorously established in certain cases [33].) Our observations of the triplet-creation model tend to support this notion, but no change in the nature of the transition in the pair-creation model has been found. As in the case of multiparticle annihilation, there seems to be an important distinction between processes mediated by pairs and by triplets. We speculate that the distinction is related to the recurrence of random walks on the line. Pairs of particles are liable to be brought together by diffusion; intersections of three random walks are comparitively rare events. In other words, diffusion is more effective in destroying three-particle clusters than pairs. A low-density active state is therefore nonviable in the triplet-creation model, under rapid diffusion.

The question remains as to how the mean-field limit is achieved in the pair-creation model, as $D\to 1$. A simple argument suggests that the diffusion rate D^* marking a crossover to mean-field behavior depends on the system size. The source of correlations is the creation process. The average time interval between creation attempts is roughly $(1-D)^{-1}$, while the time required to mix a system of size L is proportional to L^2. Equating these times yields the estimate $D^*\approx 1-\text{const}/L^2$ for large L.

In summary, we found an example of a one-component, one-dimensional model with a first-order transition into an absorbing state. The essential feature of this triplet-creation model is the competition between diffusion and cluster-mediated creation. The model has been studied via steady-state and time-dependent Monte Carlo methods and mean-field theory, and has been shown to exhibit marked hysteresis. In future work we plan to locate the tricritical point more precisely, to determine the associated scaling behavior, and to pursue a more quantitative theoretical analysis via time-dependent series expansions [34].

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