Phase transition of a two-dimensional binary spreading model

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We investigated the phase transition behavior of a binary spreading process in two dimensions for different particle diffusion strengths ($D$). We found that $N>2$ cluster mean-field approximations must be considered to get consistent singular behavior. The $N=3,4$ approximations result in a continuous phase transition belonging to a single universality class along the $D=(0,1)$ phase transition line. Large scale simulations of the particle density confirmed mean-field scaling behavior with logarithmic corrections. This is interpreted as numerical evidence supporting the bosonic field theoretical prediction that the upper critical dimension in this model is $d_c=2$. The pair density scales in a similar way but with an additional logarithmic factor to the order parameter. At the $D=0$ end point of the transition line we found directed percolation criticality.

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I. INTRODUCTION

The study of nonequilibrium phase transitions in systems with absorbing phases is an active area of research in statistical physics with applications in various other fields such as chemistry, biology, and social sciences [1]. The classification of the types of phase transition found in these systems into universality classes is, nevertheless, an incomplete task. The directed percolation (DP) universality class is the most common nonequilibrium universality class [2,3]. Directed percolation was indeed found to describe the critical behavior of a wide range of systems, despite the differences in their microscopic dynamic rules. However, the presence of some conservation laws and/or symmetries in the dynamics has been found to lead to other universality classes [4].

The pair contact process (PCP) [5] is one of the models whose (steady state) critical properties belong to the DP universality class. If the model is generalized to include single particle diffusion (PCPD or annihilation/fission model [6,7]), a qualitatively distinct situation arises since states with only isolated particles are no longer frozen and the question has been raised as to whether this would modify the universality class. A field theoretical study of the annihilation/fission model was presented long ago [7]. Unfortunately, it relies on a perturbative renormalization group analysis which breaks down in spatial dimensions $d<2$ so that the active phase and the phase transition are inaccessible to this study. The upper critical dimension $d_c$ is 2 for this bosonic theory, where multiple site occupancy is allowed, contrary to the usual lattice models and Monte Carlo simulations. A fermionic field theory is not available but it is expected to lead to $d_c=1$ [8]—therefore mean-field predictions, with some logarithmic corrections, would be seen in $d=1$ if the latter is the correct theory.

Monte Carlo, coherent anomaly [9,10], and density matrix renormalization group (DMRG) studies [6,11,12] of the 1−d PCPD model proved to be rather hard due to very long relaxation times and important corrections to scaling. Several hypotheses have been put forward in order to classify its critical behavior: single type [6,11] versus two regions of different behavior [9], parity conserving class [6], mean-field behavior, diffusion-dependent exponents. Some related models were also studied [13–18] with the aim of identifying the relevant features that determine the critical properties. The matter is not yet fully clarified, but it seems most likely that this system belongs to a distinct, not previously encountered, universality class. Park et al. [15] have also pointed out that the binary character of the particle creation mechanism, rather than parity conservation, might be the crucial factor determining the type of critical behavior of the PCPD. Higher dimensional studies of PCPD-like models are thus necessary in order to clarify their universal properties and thus contribute to a full understanding of nonequilibrium phase transitions.

In the present work we studied a two-dimensional model where particle diffusion competes with binary creation and annihilation of pairs of particles. In its nondiffusive limit, this parity-conserving version of the PCPD allows for an interpretation in terms of a unary process of particle pairs. The model is described in the following section. Cluster mean-field studies are presented in Sec. III and Monte Carlo simulations are discussed in Sec. IV. Finally we summarize and discuss our results.

II. THE MODEL

The sites of a square lattice of side $L$ are either occupied by a particle (1) or empty (0). The following dynamic rules are then performed sequentially. A particle is selected at random, and (i) with probability $D$ is moved to a (randomly chosen) empty neighbor site; with the complementary probability, and provided the particle has at least one occupied neighbor, then (ii) the two particles annihilate with probability $p$ or (iii) with probability $1−p$ two particles are added at vacant neighbors of the initial particle. The selection of neighbors is always done with equal probabilities; the updating is aborted and another particle is selected, if the chosen sites are not empty/occupied as required by the process. In reaction-diffusion language one has

$$
A \bigcirc \rightarrow A, \quad 2A \rightarrow 4A, \quad (1−p)(1−D).
$$

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It is clear that, in the absence of particle diffusion \((D=0)\), only sites that belong to a pair of occupied neighbors are active. In terms of pairs—taken as particle doublets—we have a binary process where doublets are destroyed at rate \(b\) or create new doublets at rate \(1-p\); the number of offspring is greater than or equal to 2—because new pairs may also be formed with next nearest neighbor particles—and parity of the number of doublets is not conserved. This is similar to the PCP [22] and one expects to see a phase transition, in the DP universality class, between an active phase with a finite density of pairs (at low \(p\)) and an absorbing phase without pairs (for \(p>p_c\)).

When particle diffusion is included, one has a qualitatively different situation, since configurations with only particles without neighbors are no longer absorbing—the only absorbing states are the empty lattice and the configurations with a single particle. There is parity conservation in terms of particles and the creation and annihilation mechanisms are binary. The nature of the phase transition, expected to occur at some value \(p_c(D)\), is investigated below.

### III. CLUSTER MEAN-FIELD CALCULATIONS

We performed \(N\)-cluster mean-field calculations [19,20] for this model. Since the details of the dynamics will not influence the values of the mean-field critical indices, we have considered a simpler one-dimensional version of the model where the creation takes place at the nearest and next-nearest sites to one side of the parent particle.

At the site \((N=1)\) level, the evolution of the particle density \(\rho\) (denoted by \(n\) in [6]) can be expressed as

\[
\frac{\partial \rho}{\partial t} = -2p\rho^2 + 2(1-p)\rho^2(1-\rho)^2
\]

which has the stationary solution

\[
\rho(\infty) = \frac{p-1 + \sqrt{p-p^2}}{p-1}
\]

with \(p_c = 1/2\). The pair density \(\rho_2\) \((c\) in the notation of [6]) is just the square of \(\rho\) at this level. For \(p \leq p_c\), the densities behave as

\[
\rho(\infty) \propto (p_c-p)\beta,
\]

\[
\rho_2(\infty) \propto (p_c-p)\beta_2,
\]

with \(\beta = 1\) and \(\beta_2 = 2\) leading order singularities. At the critical point

\[
\frac{\partial \rho(p=1/2)}{\partial t} = 2(p/2-1)p^3,
\]

which implies that the leading order scaling is

\[
\rho(t) \propto t^{-\alpha}, \quad \rho_2(t) \propto t^{-\alpha_2},
\]

with \(\alpha = 1/2\) and \(\alpha_2 = 1\), while in the absorbing phase

\[
\rho(t) \propto t^{-1}, \quad \rho_2(t) \propto t^{-2}.
\]

All these exponents coincide with those found for the PCPD model [6] at the same level of approximation.

In the pair \((N=2)\) approximation, the density of “1” \((\rho)\) and the “11” pair density \((\rho_2)\) are independent quantities. One can easily check that the evolution of particles can be expressed as

\[
\frac{\partial \rho}{\partial t} = -2p(1-D)\rho_2 + 2(1-D)(1-p)\rho_2
\]

\[
\times \rho_2(\rho - \rho_2) + (1-D)(1-p)\rho_2(\rho - \rho_2)
\]

while the evolution of pairs

\[
\frac{\partial \rho_2}{\partial t} = -p(1-D)\rho_2 + 2\rho_2 + (p_c - p_0)^2
\]

\[
\times (1-D)(1-p)\rho_2(\rho - \rho_2) + (1-D)(1-p)\rho_2(\rho - \rho_2).\]

Owing to the nonlinearities, we could not solve these equations analytically and had to look for numerical solutions. The critical indices thus obtained at different diffusion rates \(D\) are shown in Table I. As we can see, there are two distinct regions. For \(D > \sim 0.2\) \(p_c\) is constant and \(\beta_2 = 2\), while for \(D < \sim 0.2\) \(p_c\) varies with \(D\) and \(\beta_2 = 1\). All these results are in complete agreement with those of the PCPD model in the pair approximation.

In the \(N=3\) level approximation the situation changes, as we can see in Table I: the two distinct regions for \(D > 0\) disappear and \(\beta_2 = 2\) everywhere as found in the site approximation. At \(D = 0\), however, the particle density does not vanish at the transition but goes to \(\rho(p_c) = 0.2931\). This means that the \(N=3\) level approximation is already capable of describing the absorbing state that contains frozen, isolated particles. For \(p \leq p_c\), \(\rho - \rho(p) \propto (p_c - p)^\beta\) with \(\beta = 1\), the same critical exponent as the order parameter (the pair density); therefore we redefine Eq. (4) now. These results are also in agreement with those of the PCP model [24–26].

This kind of singular mean-field behavior persists for \(N=4\) (Table I, Fig.1) and can be found in the \(N=3,4\) level approximations of the PCPD model as well [23]. These results suggest that the \(N=2\) approximation is an odd one.
excludes the possibility of a finite size scaling study at \( t_{\text{max}} \) was measured up to \( r \)
ing the local slopes of \( a \)
the exponent \( \alpha \) is critical like \( a \).

Recent investigations in similar PCP-like models \( @24,25 \) have also shown discrepancies in the singular behavior of the low-level cluster mean-field approximations. One can conclude that in these models at least \( N>2 \) cluster approximations are necessary to find a correct mean-field behavior. It is probably just a coincidence that the \( N=1 \) calculation produced the same results. We shall thereafter ignore the \( N=2 \) results and refer to the \( N=1,3 \) scenario as the mean-field prediction.

IV. SIMULATION RESULTS

The simulations were started on small lattice sizes \( (L=100,200) \) to locate the phase transition point roughly at \( D=0, 0.05, 0.2, 0.5, 0.8 \). The particle density decay \( \rho(t) \) was measured up to \( t_{\text{max}}=60,000 \) Monte Carlo sweeps (MCS) in systems started from fully occupied lattices and possessing periodic boundary conditions. Throughout the whole paper \( t \) is measured in units of Monte Carlo sweeps. For \( D=0.05 \) we have not done such a detailed analysis as for other diffusion rates but only checked that the results are in agreement with the conclusions derived from the \( D=0.2, 0.5, 0.8 \) data.

Then we continued our survey on larger lattices \( L=400, 500, 1000, 2000, 2000 \) and determined \( p_c \) at each size by analyzing the local slopes of \( \rho(t) \):

\[
\alpha_{\text{eff}}(t) = -\frac{\ln[\rho(t)/\rho(t/m)]}{\ln(m)}
\]  

(we used \( m=8 \)). In the \( t \to \infty \) limit the critical curve goes to the exponent \( \alpha \) by a straight line, while sub- (super)critical curves veer down (up), respectively. The \( p_c(L) \) estimates exhibit an increase with \( L \); hence at the true critical-point the critical like \( \alpha_{\text{eff}} \) curves of a given \( L \) are subcritical. This excludes the possibility of a finite size scaling study at \( p_c \).

A. Dynamical scaling for \( D>0 \)

For the largest system size \( (L=2000) \) at \( D=0.5 \) diffusion rate the local slope analysis results in a \( p_c = 0.43915(1) \) and the corresponding \( \alpha = 0.50(2) \) decay exponent agrees with the mean-field value (see Fig. 2).

We also measured the pair density \( \rho_2(t) \); applying a local slope analysis similar to Eq. (11) suggests (Fig. 3) the lack of a phase transition of this quantity at \( p=0.43915 \). Instead the curves veer up, which may lead to different \( p_c \) and \( \alpha_2 \) estimates. Such strange behavior has already been observed in PCPD model simulations \( @27,28 \).

An explanation for this discrepancy was pointed out by Grassberger in the case of the PCPD model \( @28 \). Random walks in two dimensions are just barely recurrent and single particles can diffuse for a very long time before they encounter other particles. Therefore, it is natural to expect that \( \rho(t)/\rho_2(t) \sim \ln(t) \) and Fig. 4 shows that this really happens at \( p_c \).

Therefore, at \( D=0.5 \) we can conclude that \( \alpha_2 \approx \alpha = 0.5 \) taking into account logarithmic corrections. This, however, contradicts the mean-field approximation value \( \alpha_2 = 1 \).

Similar local slope analyses for \( D=0.2 \) and \( D=0.8 \) seem to imply \( \alpha = 0.46(2) \) and \( \alpha = 0.57(2) \), respectively. First this raises the idea that the exponents might change continuously with \( D \) as was observed in some one-dimensional PCPD simulations \( @9,18 \). Nevertheless, the deviations from 0.5 are small; hence we tried to fit our data including logarithmic corrections. Logarithmic corrections may really arise if \( d_c = 2 \) as predicted by bosonic field theory \( @7 \). The precise
form of these corrections is not known, however, for the present case so we have tried several functional dependences, and found that

\[ \{[a + b \ln(t)]t\}^\alpha \]  

is a good choice. As Fig. 5 shows for \( D = 0.2 \) this really works with exponent \( \alpha = 0.507 \).

Similarly, for \( D = 0.8 \) the same logarithmic formula fitting resulted in \( \alpha = 0.497 \). The coefficient of the logarithmic correction term is negative (\( b = -0.2776 \)), while it is positive for \( D = 0.2 \) (\( b = 0.468 \)).

These results suggest that logarithmic corrections to scaling should work for all cases we investigated, but at \( D = 0.5 \) they are very small and change sign. Indeed, applying the same formula for the \( D = 0.5 \), \( p = 0.43913 \) data we obtained \( \alpha = 0.496 \) with \( b = 0.00027 \) and \( a = 1.552 \). As we found logarithmic corrections to the particle density decay and a logarithmic relation between \( \rho_2(t) \) and \( \rho(t) \), we may expect even stronger logarithmic corrections to the \( \rho_2(t) \) data. Trying different forms for \( D = 0.2, 0.5, 0.8 \) we found that taking into account \( \ln^2(t) \) correction terms is really necessary, and the best choice is

\[ \{[a + b \ln(t) + c \ln^2(t)]t\}^{-\alpha}. \]  

This resulted in \( \alpha_2 = 0.5007 \) for \( D = 0.2 \) (see Fig. 5), \( \alpha = 0.501 \) for \( D = 0.5 \), and \( \alpha = 0.484 \) for \( D = 0.8 \). All these results imply that \( \alpha \approx \alpha_2 \approx 0.5 \) independently of the diffusion rate \( D \). For \( \rho(t) \) this agrees with the mean-field approximations and we do not see a change of universality by varying \( D \) as inferred from the \( N=2 \) approximation. The critical behavior of \( \rho_2(t) \), however, differs from the \( \alpha_2^{MF} = 1 \) prediction.

**B. Static behavior for \( D > 0 \)**

The \( p_c \) estimates for different sizes were used to extrapolate to the true critical value. Simple linear fitting as a function of \( 1/L \) resulted in the values given in Table II. For determining steady state exponents the densities \( \rho^L(t,p,D) \) and \( \rho_2^L(t,p,D) \) were followed in the active phase until level-off values were found to be stable. Averaging was done in the level-off region for 100–1000 surviving samples—those with more than one particle [12]. Again at each \( p \) and \( D \) we extrapolated as a function of \( 1/L \) to the \( \lim_{L \to \infty} \rho^L(\infty,p,D) \) values. The local slope analysis of exponent \( \beta \),

\[ \beta_{ef}(\epsilon_i,D) = \frac{\ln[\rho(\infty,\epsilon_i,D)] - \ln[\rho(\infty,\epsilon_{i-1},D)]}{\ln(\epsilon_i) - \ln(\epsilon_{i-1})} \]  

where \( \epsilon = p_c - p \), shows that the order parameter \( p \) exhibits \( \beta \approx 1 \) asymptotic scaling at \( D = 0.2, 0.5, 0.8 \) (Fig. 6) although a correction to scaling can be seen in all cases.

\( \beta = 1 \) agrees with the mean-field prediction. Doing the same analysis for \( \rho_2 \) the local slopes seem to extrapolate to \( \beta = 1.2 \) for each \( D \). This is very far from the mean-field value \( \beta_{MF} = 2 \) and we do not see any change by varying the diffusion rate down to \( D = 0.05 \). We have investigated the possibility of different logarithmic corrections and found that the form

\[ \rho = \epsilon^{\ell[a + b \ln(\epsilon)]^\beta} \]  

gives very good fitting with \( \beta = 0.96(5) \) for \( D = 0.5 \) while for \( D = 0.2 \) and \( D = 0.8 \) (as in the exponent \( \alpha_2 \) case) we need to take into account \( \ln^2(\epsilon) \) correction terms to obtain a similarly good fitting (see Table II and Fig. 7). Therefore we concluded that, as in the \( \alpha \) case, the steady state exponents are

**TABLE II. Summary of simulation results at criticality.**

<table>
<thead>
<tr>
<th></th>
<th>( D = 0.2 )</th>
<th>( D = 0.5 )</th>
<th>( D = 0.8 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( p_c )</td>
<td>0.4124(1)</td>
<td>0.4394(1)</td>
<td>0.4751(1)</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>0.507(10)</td>
<td>0.496(6)</td>
<td>0.497(10)</td>
</tr>
<tr>
<td>( \alpha_2 )</td>
<td>0.501(10)</td>
<td>0.501(5)</td>
<td>0.484(15)</td>
</tr>
<tr>
<td>( \beta )</td>
<td>1.07(10)</td>
<td>1.01(10)</td>
<td>1.07(10)</td>
</tr>
<tr>
<td>( \beta_2 )</td>
<td>1.03(8)</td>
<td>0.96(5)</td>
<td>0.95(5)</td>
</tr>
</tbody>
</table>
equal: $\beta = \beta_2$. Note that we have checked that logarithmic corrections to scaling can also be detected in the $r$ data with exponent $\beta \approx 1$.

**C. Data collapse for $D > 0$**

To test further the possibility of mean-field critical behavior we performed finite size scaling on our $\rho(t, p, D)$ data assuming the mean-field exponents $[7] \beta = 1$, $\nu_\perp = 1$ and the scaling form

$$\rho_L(t, \varepsilon, D) \propto L^{-\beta \nu_\|} f(\varepsilon L^{\nu_\perp}).$$  \hspace{1cm} (16)

As Fig. 8 shows, a good data collapse was obtained for $p_c = 0.4395(1)$ at $D = 0.5$.

Similarly, the scaling form

$$\rho_L(t, \varepsilon, D) \propto t^{-\beta \nu_\|} g(t \varepsilon^\nu_\perp)$$  \hspace{1cm} (17)

($\alpha = \beta \nu_\|)$ can be checked near $p_c$, assuming the mean-field values $[7] \beta = 1$ and $\nu_\| = 2$. For the largest size ($L = 2000$) at $D = 0.5$ the best collapse of curves corresponding to $p = 0.438$, 0.4382, 0.4384, 0.4386, 0.4388 was obtained for $p_c = 0.4394(1)$ (see Fig. 9). This agrees well with previous $p_c$ estimates within the margin of numerical accuracy.

**D. The $D = 0$ case**

As explained above, we expect this model to exhibit $(2 + 1)$-dimensional DP universality because for the pair density the conditions of the DP hypothesis [2,3] are satisfied. Indeed, at $p_c = 0.3709(1)$ we found that the decay exponent of pairs is $\alpha_3 = 0.45(1)$ and the steady state density approaches zero with the scaling exponent $\beta_2 = 0.582(1)$ in agreement with the estimates for this class $\alpha = 0.4505(10)$ and $\beta = 0.583(14)$ [21]. At the critical point the density of isolated particles takes a nonzero value, usually called the natural density $\rho(p_c) = 0.135$. In [26] we showed that in the case of the PCP and another 1D model exhibiting infinitely many absorbing states the nonorder field follows the scaling of the order parameter field. Here we found that the total density shows a singular behavior,

$$\rho(p) - \rho(p_c) \propto (p_c - p)_\beta.$$  \hspace{1cm} (18)

FIG. 8. Finite size data collapse according to scaling form Eq. (16) for $L = 200, 400, 500, 1000, 2000$. Different symbols denote data for $p = 0.436, 0.437, 0.4375, 0.438, 0.4382, 0.4384, 0.4386$.

FIG. 9. Data collapse according to scaling form Eq. (17) at $D = 0.5$. Different curves correspond to data at $p = 0.438, 0.4382, 0.4384, 0.4386, 0.4388$.
FIG. 10. Density decay in the inactive phase. For large times ($t > 8 \times 10^4$ MCS) we found $\rho(t) = [4.46 + 0.078(2) \ln t/t]^2$ behavior by fitting data.

with the redefined exponent $\beta = 0.60(2)$, agreeing with that of the DP class within the margin of numerical accuracy.

E. Scaling in the inactive phase

According to the bosonic field theory [7] in the inactive phase the $A + A \to \emptyset$ reaction governs the particle density decay. This process was solved exactly by Lee [29], who predicted the following late time scaling behavior in $d = 2$:

$$\rho(t) = \frac{1}{8\pi D} \ln t/t + O(1/t). \quad (19)$$

We measured $\rho(t)$ at $p = 0.45$ and $D = 0.5$ in an $L = 2000$ system up to $t_{max} = 3 \times 10^5$ MCS. As Fig. 10 shows, for intermediate times the density decays faster than this power law in agreement with results for the PCPD [28] but later crosses over to the expected Eq. (19) behavior with amplitude $0.078(2)$ and with a $4.46/t$ correction to scaling term.

Unlike what we found at the critical point (see Sec. IV B), $\rho_2(t)$ decays faster than $\rho(t)$ in the absorbing phase. The long time behavior seems to be $\rho_2 \propto t^{-2}$, which agrees with the mean-field prediction.

V. CONCLUSIONS

We have investigated the phase transition of a two-dimensional binary spreading model exhibiting parity conservation. In what concerns cluster mean-field approaches, the results are similar to those of the PCPD model at the corresponding level of approximation [6,23]. The $N = 2$ results suggest two different universality classes depending on the diffusion strength. Higher ($N = 3, 4$) order cluster mean-field calculations show a single universality class characterized by $\beta = 1$ and $\alpha = 1/2$. Comparing these with other recent results for PCP-like models and with the simulations, we believe that the $N = 2$ case yields spurious results—although two universality classes were apparently observed in a study of the one-dimensional PCPD [9]—and so $N > 2$ cluster approximations are necessary to describe the mean-field singularity correctly. This is not surprising and was already found in similar models [24,25]. Note that in both the $N = 3$ and $N = 4$ approximations, $p_c$ seems to have a discontinuity on approaching $D = 0$. This behavior may be the subject of further studies.

We performed extensive and detailed simulations along the phase transition line and found a single universality class with the order parameter exponents $\beta = 1$ and $\alpha = 0.5$ for all $D > 0$. Logarithmic corrections to scaling were detected that are weakest at $D = 0.5$. Lacking theoretical prediction, we have selected the best logarithmic fitting forms taking into account up to $O(\ln^2)$ terms, but we cannot rule out the possibility of other forms of logarithmic correction. Scaling function analysis confirmed the $\nu_1 = 2$ and $\nu_2 = 1$ mean-field values. This seems to indicate that the critical dimension is $d_c = 2$ as predicted by the bosonic field theory. In the inactive region, the decay of particle density at large times was found to agree with an exact prediction [29].

The pair density $\rho_2$ for $p < p_c$ (where the bosonic field theory breaks down) was shown to exhibit the same singular behavior as the order parameter, apart from a logarithmic ratio. Simulation results of the PCPD model [28,10] found indications of similar behavior. The reason why the mean-field approximation fails to describe the singular behavior of $\rho_2$ is not yet clear to us, but in the two-component description of the model it indicates strong coupling between pairs and particles (similarly to other models [5,31,30]). In the inactive region, however, $\rho_2$ and $\rho$ scale differently. At the $D = 0$ end point of the transition line we found $(2 + 1)$-dimensional DP critical behavior of $\rho_2$ with infinitely many frozen absorbing states, similar to the PCP model.

We have found identical predictions for the present and the PCPD model within the mean field, which seem to be confirmed by our simulations—and also by preliminary simulations for the $2 - d$ PCPD [27,28]. One thus concludes that it is very likely that parity conservations is irrelevant for this transition, as in the one-dimensional case [15] and in certain models with exclusion [32]. Further renormalization group studies of these systems are necessary for a proper justification of these results.

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We found that on considering samples with surviving pairs the results do not change but the logarithmic corrections become even more apparent.

[27] H. Hinrichsen (private communication).
[28] P. Grassberger (private communication).