CYCLICALLY COUPLED SPREADING AND PAIR ANNIHILATION

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Abstract. Recently it has been shown that the transition of the 1+1-dimensional annihilation-fission process \(2X \rightarrow 3X, 2X \rightarrow \emptyset\) exhibits an unusual type of nonequilibrium critical behavior. The phenomenological properties of critical clusters are characterized by two different dynamic modes for spreading and diffusion. In order to describe the interplay of these modes, we introduce an effective model which involves two species of particles \(A\) and \(B\). The \(A\)-particles perform an ordinary directed percolation process while the \(B\) particles diffuse and annihilate. Both subsystems are cyclically coupled by particle transmutation \(A \leftrightarrow B\). The resulting critical behavior is in many respects similar to the one observed in the annihilation-fission process.

1. Introduction

The study of phase transitions into absorbing states is a fascinating field of nonequilibrium statistical physics \[1\]. Such phase transitions can be observed in models for the spreading of some (generally non-conserved) agent as a result of a competition between local reproduction and decay. If the rate for reproduction is sufficiently high, the system is able to maintain a fluctuating active phase where the stationary concentration of the spreading agent is positive. On the other hand, if the decay process dominates, the concentration of the spreading agent decreases and tends to zero. Eventually the system becomes trapped in an absorbing state from where it cannot escape. An interesting situation emerges at the borderline between survival and extinction. Here the system undergoes a nonequilibrium phase transition which is characterized by non-trivial critical behavior. It is believed that transitions into absorbing states can be categorized into a finite number of universality classes. Typically each class is associated with certain symmetry properties of the dynamics.

At present two universality classes are firmly established. The first and most prominent one is the universality class of directed percolation (DP) \[2–4\]. The DP class is characterized by the absence of symmetries (apart from conventional symmetries such as translation and reflection invariance) and covers a wide range of models \[4\]. Roughly speaking, DP models follow the reaction-diffusion scheme \(X \rightarrow 2X, X \rightarrow \emptyset\). In addition, there has to be a nonlinear mechanism which limits the particle density. In ‘fermionic’ models with at most one particle per site, the density is limited automatically. In ‘bosonic’ models, allowing for infinitely many particles per site, this mechanism has to be implemented by adding the reaction \(2X \rightarrow X\). It is important to note that DP is a unary spreading process, i.e., individual particles are able to reproduce and destruct themselves.

Some time ago Grassberger et al. \[7,8\] discovered a second universality class which can be considered as a generalization of directed percolation from one to two absorbing states related by an exact \(Z_2\)-symmetry (DP2). It comprises various models, including nonequilibrium Ising models \[3\], certain monomer-dimer models \[10\], as well as generalized versions of the Domany-Kinzel model and the contact process \[11\]. In 1+1 dimensions it is possible to regard kinks between differently oriented absorbing domains as particles.
By definition, these particles evolve according to a parity-conserving dynamics, exemplified by branching-annihilating random walks with two offspring \( X \rightarrow 3X, \ 2X \rightarrow \emptyset \) \cite{12–14}. For this reason, the universality class is often referred to as the parity-conserving (PC) class. However, it should be noted that the PC class and the DP2 class are different in higher dimensions.

Three years ago, Howard and Täuber \cite{15} raised the question whether there might exist a third universality class of models with a phase transition from ‘real’ to ‘imaginary’ noise. As a prototype, they introduced the annihilation-fission (AF) process \( 2X \rightarrow 3X, \ 2X \rightarrow \emptyset \) with single-particle diffusion. Obviously, this process is neither parity-conserving nor invariant under any other unconventional symmetry transformation. In contrast to DP and DP2, the AF model is a binary process, i.e., only pairs of particles can decay or reproduce themselves. The critical properties at the transition are still poorly understood. Recently, Carlon et. al. analyzed the transition using density matrix renormalization group techniques \cite{16}. Estimating the critical exponents they arrived at the conclusion that the transition of the AF process should belong to the DP2 universality class, although there is no \( Z_2 \) symmetry or parity conservation law. However, as pointed out in Ref. \cite{17}, various physical arguments suggest that the AF process might belong to an independent universality class which has not been investigated before.

Since the universality class could not be identified so far, it is of interest to understand the most salient features of the transition in the AF process from a descriptive point of view. To this end, we introduce an effective model which separates the dynamics of pairs and solitary particles in the AF process by introducing two species of particles \( A \) and \( B \). The \( A \)'s perform an ordinary DP process while the \( B \)'s are subjected to an annihilating random walk. Both subsystems are cyclically coupled by particle transmutation. It is shown that this three-state model exhibits a nonequilibrium phase transition which is similar to the one observed in the AF process.

The following Section briefly summarizes the phenomenological properties of the AF process. In Sec. 3 we demonstrate that the critical behavior is governed by two competing dynamic modes for spreading and diffusion. Based on this interpretation we introduce an effective model involving two species of particles (see Sec. 4). In Sec. 5 the critical exponents of this model are estimated by Monte Carlo simulations. The article ends with several concluding remarks in Sec. 6.

2. Phenomenological properties of the annihilation-fission process

Assuming the usual scaling picture for phase transitions into absorbing states, we expect the AF process to be characterized by four critical exponents \( \beta, \beta', \nu_\perp, \) and \( \nu_\parallel \). The first one is associated with the field-theoretic annihilation operator and describes the behavior of the stationary density \( \rho_{\text{stat}} \sim (p-p_c)^\beta \) close to the transition. The exponent \( \beta' \) is associated with the creation operator and plays a role whenever initial conditions are specified. For example, the survival probability of a cluster grown from a single seed involves the exponent \( \delta' = \beta'/\nu_\parallel \). The other two exponents are related to the spatial and temporal correlation lengths \( \xi_\perp \sim |p-p_c|^{-\nu_\perp} \) and \( \xi_\parallel \sim |p-p_c|^{-\nu_\parallel} \), respectively. It should be noted that in the case of DP the two order parameter exponents \( \beta \) and \( \beta' \) coincide because of a duality symmetry (see e.g. Ref. \cite{4}). In the present case, however, they turn out to be different.

Using a density matrix renormalization group approach, Carlon et. al. estimated the critical exponents of the AF process for various diffusion rates \( 0.1 \leq d \leq 0.2 \). Since their estimates \( z = 1.73 \ldots 1.81 \) and \( \beta/\nu_\perp = 0.46 \ldots 0.5 \) were in fair agreement with the numerical values of DP2 exponents (see Table 1), they concluded that the AF process should belong to the DP2 universality class, although there is no \( Z_2 \)-symmetry or parity conservation law in the system. This conclusion, however, collides with the general belief that critical phenomena are determined by their symmetry properties or, equivalently, by their
associated field theories. Without the required symmetries on the microscopic level, a special mechanism would be necessary in order to restore these symmetries effectively on large scales. As there is no such mechanism, it is near at hand to expect that the AF process does not belong to the DP2 class. To support this point of view, preliminary Monte-Carlo simulations were presented in Ref. [18] and later improved by Grassberger and Ódor [19]. Because of strong corrections to scaling, the estimates for the critical exponents depend on the numerical effort. The estimates for $\delta = \nu_\perp / \nu_\parallel$, for example, are scattered over the range $0.25 \ldots 0.29$ and seem to decrease with increasing simulation time. A similar tendency was observed for the exponents $z$ and $\beta$. Moreover, it is not yet fully clear to what extent the exponents depend on the diffusion rate $d$. A tentative list of critical exponents, including recent results obtained by simulations on parallel computers [20], is given in Table 1.

In order to understand the transition in the annihilation-fission process from a phenomenological point of view it is helpful to analyze the spatio-temporal structure of critical clusters. To this end we introduce a novel type of scale-invariant space-time plot which can be used to visualize the scaling properties of critical clusters in systems with absorbing states. Starting with a localized seed (a pair of particles) at the origin and simulating the spreading process up to $10^6$ time steps, the rescaled position of the particles $x/t^{1/z}$ is plotted against $\log_{10} t$, where $z = \nu_\parallel / \nu_\perp$ is the dynamic exponent of the process under consideration (see Fig. 1). By rescaling the spatial coordinate $x$, the cluster is confined to a strip of finite width. Compared to linear space-time plots the scale-invariant representation of a cluster has several advantages. On the one hand, it is possible to survey more than four decades in time. On the other hand, the plot provides a simple visual check of scaling invariance. Roughly speaking, scaling invariance is fulfilled if the cluster’s appearance is time-independent, i.e., spatio-temporal patterns should look similar in the upper and lower parts of the figure. It is needless to say that this visual check does not replace an accurate quantitative analysis. Nevertheless such a scale-invariant plot may improve the intuitive understanding of the asymptotic long-time behavior and may also help to identify relevant and irrelevant contributions.

Let us first consider a critical cluster of a branching-annihilating random walk with two offspring (see left part of Fig. 1). Obviously, this process is characterized by an ongoing competition between particle reproduction and decay. Contrarily, the annihilation-fission process admits undisturbed random walks of solitary particles over long distances. As shown in the middle of Fig. 1, this leads to a very different visual appearance of the cluster. It is important to note that these differences persist as time proceeds. However, if both processes were to converge to the same type of long-range critical behavior as suggested in [16], we would expect the clusters to become increasingly similar in the lower part of the figure. As there is no indication of such a convergence, Fig. 1 supports the viewpoint of Refs. [17, 20] that the AF process might represent a new type of nonequilibrium critical behavior. The corresponding universality class should be characterized by the following properties:

| class/model | $\beta$   | $\delta$   | $z$      | $\delta'$ | $\eta$  |
|-------------|-----------|------------|----------|-----------|---------|
| DP          | 0.2765    | 0.1595     | 1.581    | 0.1595    | 0.3137  |
| DP2/PC      | 0.92(2)   | 0.286(2)   | 1.74(2)  | 0.286(2)  | 0 or 0  |
| AF $d = 0.1$| 0.57...0.62| 0.25...0.29| 1.67...1.83| 0.12...0.15| $\approx 0.10$ |
| AF $d = 0.5$| 0.38...0.42| 0.21...0.23| $\approx 1.7$| $\approx 0.145$| $\approx 0.23$ |
| AF $d = 0.9$| 0.38...0.40| $\approx 0.20$| $\approx 0.20$| $\approx 0.48$| $\approx 0.48$ |
| present model | 0.38(6)   | 0.21(1)    | 1.75(10) | 0.15(1)   | 0.21(2) |

Table 1. Estimates for the critical exponents in 1+1 dimensions.
Figure 1. Critical clusters generated from a single seed at the origin in a scale-invariant representation. The rescaled position $x/t^{1/z}$ of the particles is plotted against time on a logarithmic scale. The curved lines mark the positions $x = \pm 10, \pm 100$, and $\pm 1000$, respectively. Left: Branching-annihilating random walk with two offspring (BAW2). Middle: Annihilation-fission process (also called pair contact process with diffusion). Right: Cyclically coupled spreading and annihilation processes as an effective model for the AF process. The figure is explained in the text.
1. Single particles diffuse but do not react.
2. Reproduction requires two particles to meet at neighboring sites.
3. Particles are removed if at least two particles meet at neighboring sites.
4. There is no unconventional symmetry (such as parity conservation).
5. There is no frozen disorder in the system.
6. There is a mechanism limiting the density of particles.

Consequently, many other processes, such as the fission-coagulation model $2X \rightarrow 3X$, $2X \rightarrow X$ and the reaction-diffusion process $2X \rightarrow 3X$, $3X \rightarrow X$ are expected to exhibit the same type of nonequilibrium critical behavior.

3. Interpretation as a spreading process with two species of particles

To what extent is the transition in the AF model different from ordinary DP and DP2 transitions? As Fig. 1 suggests, there are two separate dynamic modes for spreading and diffusion. The spreading mode is characterized by sudden avalanches with a high density of particles. Here the dynamic processes are dominated by interacting pairs of particles. Once an avalanche has stopped, the system enters the diffusive mode, in which solitary particles perform a simple random walk. When two of them meet at neighboring sites, they may release a new avalanche, as illustrated in Fig. 2. The asymptotic critical behavior at the transition will depend on the relevance of the two dynamic modes. In principle there are three possibilities. If the spreading mode becomes dominant we expect a crossover to DP. Conversely, if the diffusive mode governs the asymptotic regime, we expect a purely diffusive behavior with the dynamical critical exponent $\gamma = 2$. However, Fig. 1 strongly suggests that both modes are equally important and balance one another as time proceeds. In fact, in the rescaled representation the typical spatio-temporal patterns do not change over four decades in time.

In order to investigate this transition in more detail, we suggest a phenomenological explanation of the observed spatio-temporal patterns. The basic idea is to describe the two dynamic modes in terms of two separate reaction-diffusion processes involving two different species of particles $A$ and $B$. The spreading

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure2.pdf}
\caption{Cartoon of three different 1+1-dimensional spreading processes. Solid (hollow) circles denote reproduction (decay) of particles. Left: Directed percolation. Middle: Parity-conserving branching annihilating random walk with two offspring. Right: Schematic drawing of the annihilation-fission process where spreading occurs in avalanches (represented as triangles) followed by diffusion of solitary particles (see text).}
\end{figure}
mode is governed by the dynamics of A-particles. Roughly speaking, the A-particles can be thought of as representing pairs of particles in the original model. Obviously, there is no parity conservation law for the number of pairs, hence the A-particles in the new model evolve effectively in the same way as in an ordinary DP process. During the avalanche, several A’s transmute into B’s. Therefore, once the avalanche has stopped, several B-particles are left behind. These B-particles in turn perform a simple random walk, representing solitary particles in the original model. When two B-particles meet, they may trigger a new avalanche of A-particles. The corresponding reaction-diffusion scheme reads

\[ A \leftrightarrow 2A, \quad A \rightarrow \emptyset, \quad 2B \rightarrow A. \] (1)

Thus the model consists of two subsystems A and B. Subsystem A is a DP process \( A \leftrightarrow 2A, A \rightarrow \emptyset \) which is coupled via transmutation \( A \rightarrow B \) to subsystem B. In this subsystem the B-particles diffuse until they annihilate and release a new avalanche of A-particles. Thus, the reaction-diffusion model (1) can be interpreted as a cyclically coupled sequence of a DP and a pair annihilation process, as sketched in Fig. 3. It should be pointed out that Figs. 2-3 are over-simplified in the sense that they suggest the existence of strictly separated dynamic modes. In reality, however, the two modes are not completely separated, rather they are entangled and sustain each other in an intricate manner. Nevertheless it is the hope of the present study that the AF-process and the simplified reaction-diffusion scheme (1) exhibit at least qualitatively a similar type of nonequilibrium critical behavior.

4. A LATTICE MODEL FOR CYCLICALLY COUPLED DIRECTED PERCOLATION AND PAIR ANNIHILATION

In order to study the process (1) quantitatively, we introduce a three-state model on a square lattice with random-sequential updates which is defined by the following dynamic rules:

- **reproduction:**
  - \( \emptyset A \rightarrow AA \) with rate \( p/2 \)
  - \( BA \rightarrow AA \) with rate \( p/2 \)
  - \( AO \rightarrow AA \) with rate \( p/2 \)
  - \( AB \rightarrow AA \) with rate \( p/2 \)

- **decay:**
  - \( A \rightarrow \emptyset \) with rate \( (1-p)(1-\tau) \)

- **transmutation:**
  - \( A \rightarrow B \) with rate \( (1-p)\tau \)

- **diffusion:**
  - \( \emptyset B \leftrightarrow B \emptyset \) with rate \( D/2 \)

- **annihilation:**
  - \( BB \rightarrow AO \) with rate \( r/2 \)
  - \( BB \rightarrow OA \) with rate \( r/2 \)

In the following the numerical analysis will be restricted to the case \( r = D = 1 \). Thus, the model is controlled by two parameters, namely the rate for particle reproduction \( p \) and the transmutation rate \( \tau \).
Obviously, the model has two absorbing states, i.e., the empty lattice and the state with a single diffusing $B$-particle. The phase diagram in Fig. 4 comprises two phases. For low values of $p$ and $\tau$, the system is in the inactive phase where it approaches one of the two absorbing states. If $p$ and $\tau$ are sufficiently large, an active steady state with non-vanishing particle densities $\rho_A$ and $\rho_B$ exists on the infinite lattice. Here we are interested in the critical behavior at the phase transition line. It should be noted that the case $p = 0$ is special. In this case the spreading process does not generate $B$ particles. Hence, starting with $A$-particles, the critical behavior belongs to the DP universality class. For $p > 0$, however, we observe non-DP critical behavior. In fact, an ordinary DP transition seems to be unlikely since the inactive phase is characterized by an algebraic decay of the particle density. Similarly, we can rule out the possibility of a DP2 transition since there is neither a $Z_2$-symmetry nor a parity conservation law in the model.
5. Numerical results

In order to estimate the critical exponents in 1+1 dimensions, we perform Monte Carlo simulations. Starting with randomly distributed A’s and B’s, we first measure the densities ρ_A(t) and ρ_B(t) up to 3·10^5 time steps. As can be seen in the left panel of Fig. 5, the ratio ρ_B(t)/ρ_A(t) approaches a constant value. Assuming an algebraic decay, both quantities should therefore scale with the same critical exponent

\[ \rho_A(t) \sim \rho_B(t) \sim t^{-\delta}. \]

The temporal decay of the particle densities is shown in the right panel of Fig. 5. As in the case of the AF model, we observe strong corrections to scaling, leading to a considerable curvature of the data. However, compared to the AF model these corrections are less severe. Moreover, the curvatures for ρ_A and ρ_B have opposite signs. Thus, the local slopes approach the postulated ‘true’ value of δ from both sides. Seeking for the best compromise, we are able to estimate the critical points by

\[
\begin{array}{c|c|c|c|c}
\tau & 0 & 0.1 & 0.5 & 1 \\
\hline
p_c & 0.7674(3) & 0.757(2) & 0.6920(1) & 0.540(1) \\
\end{array}
\]

For \( \tau = 0.5 \) the corresponding exponent is given by \( \delta = \beta/\nu_\parallel = 0.21(2) \). Similar measurements for \( \tau = 0.1 \) and \( \tau = 1 \) (not shown here) suggest that this value is the same for all \( \tau > 0 \). In order to obtain the dynamic exponent \( z = \nu_\parallel/\nu_\bot \), we perform finite size simulations at criticality. Here the particle densities should obey the scaling form

\[ \rho_A(t) \sim \rho_B(t) \sim t^{-\delta} f(t/L^z), \]

where \( f \) is a universal scaling function. Thus, plotting \( \rho t^\delta \) against \( t/L^z \), all data sets should collapse onto a single curve. Comparing different data collapses it turns out that \( \rho_B \) shows a much cleaner scaling behavior than \( \rho_A \). As shown in Fig. 6, the best collapse is obtained for \( \delta = 0.215(15) \) and \( z = 1.75(5) \).

To obtain the third exponent, we study the behavior \( \rho_B(t) \) below and above criticality. According to the usual scaling theory for absorbing-state transition, we expect the scaling form

\[ \rho_B(t) \sim t^{-\delta} g(t^{\epsilon_\parallel}), \]
where $\epsilon = |p - p_c|$ denotes the distance from criticality. Plotting $\rho_B(t)t^\delta$ against $t^{\epsilon\nu_\parallel}$ (see Fig. 3), the best data collapse is obtained for $\delta = 0.215(20)$ and $\nu_\parallel = 1.8(1)$.

In order to cross-check these estimates, we perform dynamic simulations starting with a single pair of particles located in the center [21]. As usual in this type of simulations, we measure the survival probability $P(t)$ that the system has not yet reached one of the two absorbing states, the average numbers of particles $N_A(t)$ and $N_B(t)$, and the mean square spreading of all particles from the origin $R^2(t)$ averaged over the surviving runs. Assuming that $N_A(t)$ and $N_B(t)$ scale asymptotically with the same exponent, these quantities should obey the power laws

$$P(t) \sim t^{-\delta'}, \quad N_A(t) \sim N_B(t) \sim t^\eta, \quad R^2(t) \sim t^{2/z}$$

with certain dynamical exponents $\delta'$ and $\eta$. As shown in Fig. 7, the survival probability shows a clean power law over almost five decades. Moreover, the quotient $N_B(t)/N_A(t)$ quickly tends to a constant value. Fitting power laws to the data shown in Fig. 7, we obtain the estimates

$$\delta' = 0.15(1), \quad \eta = 0.21(1), \quad 2/z = 1.16(4).$$

Together with the previous results these estimates satisfy the generalized hyperscaling relation [22]

$$\delta + \delta' + \eta - d/z = 0$$

within numerical errors. Combining all results, the critical exponents are given by

$$\beta = 0.38(6), \quad \beta' = 0.27(3),$$

$$\nu_\parallel = 1.8(1), \quad \nu_\perp = 1.0(1).$$

It should be noted that the error bars were obtained by assuming power-law behavior. Thus, they do not include systematic errors due to possible corrections to scaling emerging after very long time.
6. Conclusions

This work was motivated by recent studies of the annihilation-fission process which exhibits a novel type of nonequilibrium critical behavior. Using a scale-invariant space-time plot we have demonstrated that critical clusters of the AF process are characterized by an interplay of two different dynamic modes. In the high-density mode we observe spreading avalanches whereas the low-density mode is characterized by random walks of solitary particles. In order to understand the interplay between these modes from a phenomenological point of view, we have introduced an effective model which involves two species of particles. The dynamic rules of this model can be regarded as being composed of cyclically coupled DP and pair annihilation processes, i.e., it follows the reaction-diffusion scheme $A \leftrightarrow 2A$, $A \to B$, $2B \to A$. The model exhibits a nonequilibrium phase transition which is in many respects similar to the one observed in the AF process. In fact, the AF process and the three-state model proposed in the present work have several features in common:

- They both have two non-symmetric absorbing states, namely the empty lattice and the state with a single diffusing particle.
- There is no unconventional symmetry (such as parity conservation).
- Both models exhibit a continuous nonequilibrium phase transition with non-DP critical exponents.
- The visual appearance of critical clusters is very similar (see Fig. 1).

Compared to the AF process, the three-state model has several advantages. On the one hand, it is defined as a two-site nearest neighbor process. On the other hand, corrections to scaling are less severe, allowing us to determine the critical exponents more accurately.

There are several open questions. Is the critical behavior of the three-state model universal? If this is indeed the case, does it represent a independent universality class different from DP and DP2? Are the AF process and the present model in the same universality class, i.e., do they have the same critical exponents? From the field-theoretic point of view, there is no reason for them to coincide. Yet the two classes may ‘intersect’ in 1+1 dimensions. Very recently, Ődor carried out a systematic study of the annihilation/fission process performing simulations on a parallel computer combined with generalized mean field approximations and coherent anomaly extrapolations [20]. He reports two different universality classes for low and high values of the diffusion constant $d$. The corresponding critical exponents are shown in Table 1. According to Ődor, the exponents for $d \geq 0.5$ are in fair agreement with the exponents observed in the three-state model. However, this conclusion is still speculative and needs to be substantiated by further investigations.

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