

## Phase transition of triplet reaction-diffusion models

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The phase transitions classes of reaction-diffusion systems with multiparticle reactions are an open challenging problem. Large scale simulations are applied for the  $3A \rightarrow 4A$ ,  $3A \rightarrow 2A$  and the  $3A \rightarrow 4A$ ,  $3A \rightarrow \emptyset$  triplet reaction models with site occupation restriction in one dimension. Static and dynamic mean-field scaling are observed with signs of logarithmic corrections suggesting  $d_c=1$  upper critical dimension for this family of models.

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### I. INTRODUCTION

The exploration of the universal behavior of nonequilibrium phase transitions is still an open problem of statistical physics [1–3]. In equilibrium critical phenomena symmetries, dimensions and boundary condition are the relevant factors determining a universality class. During the study of nonequilibrium models other circumstances like initial conditions or topological effects in low dimensions have been proven to be decisive [4]. Unfortunately a solid field theoretical background exists for only a few reaction-diffusion (RD) systems exhibiting continuous phase transition to absorbing states [5]. These are mainly branching and annihilating random walk models  $A \rightarrow (n+1)A$ ,  $2A \rightarrow \emptyset$  built up from unary particle creation [6–8] RD models are interesting since many other types of systems like surface growth, spin systems or stochastic cellular automata can be mapped on them [3].

Recently RD systems with multiparticle creation have become the focus of research. Numerical studies resulted in debated critical phenomena and generated a long series of publications. An interesting example was being investigated during the past decade that emerges at the phase transitions of binary production systems (PCPD) [9]. In these systems particle production competes with pair annihilation and single particle diffusion. If the production wins steady states with finite particle density appearing in (site restricted) models with hard-core repulsion, while in unrestricted (bosonic) models the density diverges. If the annihilation is stronger an absorbing phase emerges, which is either completely empty or contains a solitary diffusing particle. In between the two phases a continuous phase transition can be observed in site restricted models.

In triplet reaction models at least three particles are needed to contact for a reaction. They have been investigated by simulations [10–12] and a numerical Langevin equation solution [15]. The first simulation results [10,11] for  $3A \rightarrow 4A$ ,  $3A \rightarrow 2A$  models in one dimension claimed a distinct universal behavior from the known ones. Simple power-counting analysis of an effective Langevin equation corresponding to the coarse grained microscopic model results in  $d_c=4/3$  [12]. However, the numerical estimates for the critical exponent describing the density decay from homogeneous random initial state  $\rho(t) \propto t^{-\alpha}$  differed significantly  $\alpha=0.32(1)$  [10] vs  $\alpha=0.27(1)$  [11]. In the former case a site

restricted model was investigated and scaling was reported in the  $10^4 < t < 10^6$  region. In Ref. [11] different suppressed bosonic triplet models—where the multiple site occupancy is suppressed by an exponential probability factor—exhibited scaling for  $10^4 < t < 10^7$  Monte Carlo steps (MCS) (throughout the paper the time is measured by MCS). Renormalization group analysis pointed out [16] that a single field theory does not exhibit a nontrivial stable fixed point and suggested  $d_c=1$  for such models. This study raised the possibility that a proper field theory should be a coupled one, with positively correlated clustered particles and solitary random walkers. Another simulation study [12] on site restricted models reported scaling agreeing with mean-field exponents  $\alpha=0.33(1)$  and  $\beta=1.07(10)$ , where  $\beta$  is the order parameter exponent in the active phase  $\rho \propto |p-p_c|^\beta$ .

Very recently a coupled field theoretical description of such systems is suggested [15]. An effective Langevin equation between a directed percolation (DP) like and an annihilating random walk (ARW) system is analyzed by the numerical integration technique. Note, however, the ARW like system is described by a positive noise term saying that at the critical point the anticorrelations do not play a role and serve merely as a fluctuating source to the primary field. As a consequence, this field theory leads to the same critical scaling behavior as that of the PCPD albeit with a different upper critical dimension  $d_c=4/3$  (versus  $d_c=2$  for PCPD). So according to this study in one dimension one should see PCPD class exponents:  $\alpha=0.20(1)$  and  $\beta=0.40(1)$  [11,17].

In the present study I extend the simulation time of the  $3A \rightarrow 4A$ ,  $3A \rightarrow 2A$  model investigated in Ref. [12] by two orders of magnitude and follow the static and dynamic scaling behavior of particles and triplets (AAA) at different diffusion probabilities. In Sec. (3) I apply the same kind of analysis for the  $3A \rightarrow 4A$ ,  $3A \rightarrow \emptyset$  model.

### II. SIMULATIONS OF THE $3A \rightarrow 4A$ , $3A \rightarrow 2A$ MODEL

The simulations were carried out on  $2 \times L=10^5$  sized systems with periodic boundary conditions. The initial states were randomly half filled lattices, and the density of particles, singlets, and triplets is followed up to  $2 \times 10^9$  MCS by random sequential dynamics. An elementary MCS consists of the following steps. A particle  $A$  is chosen randomly and the following processes are done:

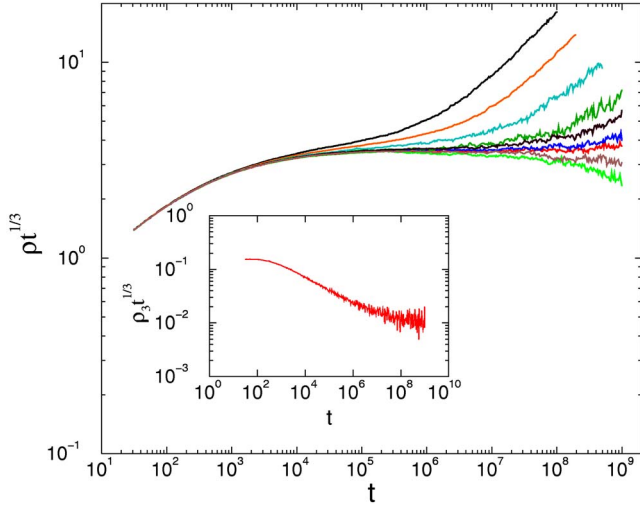


FIG. 1. (Color online) Density decay of the  $3A \rightarrow 4A$ ,  $3A \rightarrow 2A$  model at  $D=0.1$ . Different curves correspond to  $p=0.301, 0.302, 0.3027, 0.3031, 0.3032, 0.3033, 0.30335, 0.3034, \text{ and } 0.3035$  (from top to bottom). The inset shows the decay of triplets:  $\rho_3 t^{1/3}$ , for  $p=0.30337$

- (a)  $A \emptyset \leftrightarrow \emptyset A$  with probability  $D$ ,
- (b)  $3A \rightarrow 2A$  with probability  $p(1-D)$ ,
- (c)  $3A \rightarrow 4A$  with probability  $(1-p)(1-D)$ ,

such that the reactions were allowed on the left or right side of the selected particle strings randomly. The time—measured by MCS—is updated by  $1/n_p$ , where  $n_p$  is the total particle number at time  $t$ . In order to get precise  $\rho(t)$ , the critical point and exponent estimates the number of independent realizations varied between 20 and 350 per  $p$  and  $D$  throughout this study.

First, I extended the simulations at  $D=0.1$  published in Ref. [12] from  $t_{\max}=10^7$  MCS by a factor of 200 in time. Figure 1 shows the density decay multiplied by  $t^{1/3}$ . Following a long initial transient, where the decay is slow an excellent agreement with the mean-field scaling can be observed for  $10^6 < t < 10^9$  MCS for  $p_c=0.30337(2)$ . The triplet density decays in the same way ( $\rho_3 \propto t^{1/3}$ ) as the total density suggesting  $d_c=1$ .

I repeated the simulations for a higher diffusion rate  $D=0.8$  (Fig. 2). In this case due to the dynamics of this model the reaction rates are smaller and one can observe a faster than mean-field decay for  $10^4 < t < 5 \times 10^8$  MCS. Agreement with mean-field scaling sets in for  $5 \times 10^8 < t < 2 \times 10^9$  MCS steps for  $p=0.4075(1)$ . Fast transient decay for intermediate times has already been explained in case of the  $AA \rightarrow A$  coagulation model with finite reaction rates [13,14]. One may expect similar behavior for the triplet annihilation case where the low reaction rates at  $D=0.8$  can explain the fast transient seen here. Again, the triplet density decays by the mean-field law for  $t > 5 \times 10^8$  MCS as expected at the upper critical dimension  $d_c=1$ . Using the critical point estimates obtained by the dynamical simulations I investigated the singular behavior of the order parameter in the supercritical region as well. The order parameter is expected to scale as

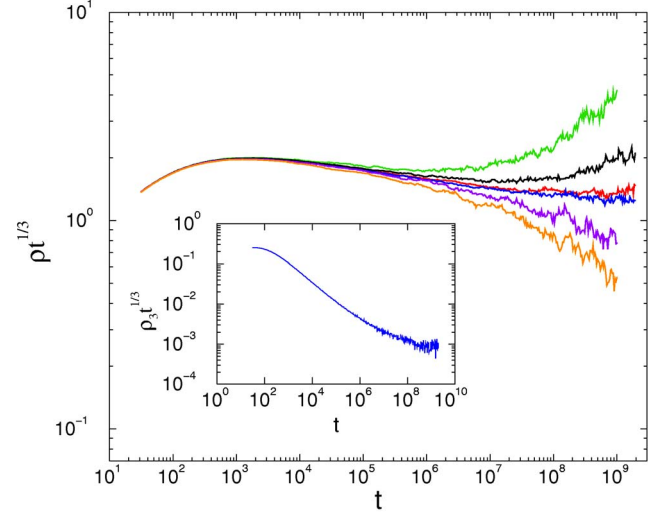


FIG. 2. (Color online) Density decay of the  $3A \rightarrow 4A$ ,  $3A \rightarrow 2A$  model at  $D=0.8$ . Different curves correspond to  $p=0.406, 0.407, 0.4074, 0.4075, 0.408, \text{ and } 0.409$  (from top to bottom). The inset shows the triplet density decay at  $p=0.4075$ .

$$\rho \propto |p - p_c|^\beta. \quad (1)$$

To get the steady state densities I followed the decay in several samples until saturation occurs and averaged it in a long time window exceeding a level-off seen on log-lin scale. The data are analyzed by the local slopes method. According to this

$$\beta_{\text{eff}}(p_i) = \frac{\ln \rho(\infty, p_i) - \ln \rho(\infty, p_{i-1})}{\ln(p_i) - \ln(p_{i-1})}, \quad (2)$$

and as  $p_i \rightarrow p_c$  the effective exponent tends to the true critical value  $\beta_{\text{eff}} \rightarrow \beta$ . As Fig. 3 shows the  $\beta_{\text{eff}}$  converges to the

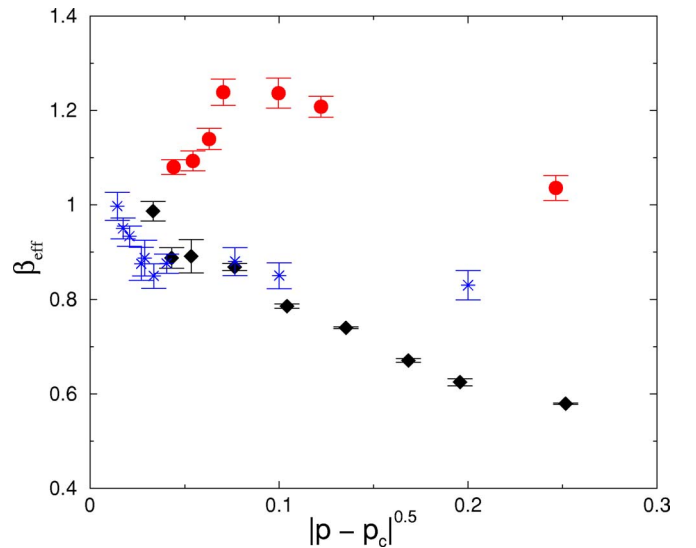


FIG. 3. (Color online) Effective static order parameter exponent results in the active phase. Bullets correspond to  $D=0.8$ , boxes to  $D=0.1$  of the  $3A \rightarrow 4A$ ,  $3A \rightarrow 2A$  model. Stars denote the results of the  $3A \rightarrow 4A$ ,  $3A \rightarrow \emptyset$  model.

mean-field value  $\beta=1$  for both diffusion rates I investigated. For  $D=0.8$  one can see an overshooting, while for  $D=0.1$  local slopes approach the asymptotic value from below following an upward curvature. This kind of effective exponent behavior usually corresponds to logarithmic correction to scaling. In the case of the general form

$$\rho(\infty) = \epsilon^\beta \ln^x(\epsilon), \quad (3)$$

where  $\epsilon=|p-p_c|$ , the effective exponent behaves as

$$\beta_{eff} = \frac{d \ln[\rho(\infty)]}{d \ln(\epsilon)} = \beta + \frac{x}{\ln(\epsilon)}. \quad (4)$$

Applying this form to the data of Fig. 3 one obtains:  $\beta=1.05(5)$ ,  $x=1.2(1)$  for  $D=0.1$  and  $\beta=0.93(10)$ ,  $x=-1.1(1)$  for  $D=0.8$ . Although the assumed scaling correction form may look somewhat ad hoc it indicates  $d_c=1$ .

I also considered the scenario suggested by Ref. [15] according to which PCPD scaling  $\{\alpha=0.19(1)$  [17,15] $\}$  should be observed at the transition point. By assuming that such density decay appears for very long times ( $t > 10^9$  MCS) one can read-off the corresponding slightly different critical point estimates:  $p_c=0.303\,25(5)$  for  $d=0.1$  and  $p_c=0.4071(1)$  for  $D=0.8$ . Using these values in the local slopes analysis one can obtain:  $\beta=0.85(5)$  for  $D=0.1$  and  $\beta=0.80(5)$ , neither of them is near to the exponent  $\beta=0.40(1)$  of the PCPD class [17]. Therefore these simulations can not support the PCPD class scenario.

### III. SIMULATIONS OF THE $3A \rightarrow 4A$ , $3A \rightarrow \emptyset$ MODEL

Considering the mean-field type of scaling behavior of the  $3A \rightarrow 4A$ ,  $3A \rightarrow 2A$  model one may speculate that in this model the spatial fluctuations are somewhat suppressed: it is hard to create nearly arbitrarily large regions void of particles from a place where ‘‘annihilation’’ reactions have taken place due to the  $3A \rightarrow 2A$  rule. In the low-diffusion regime, when a particle was created from the configuration  $\cdots 0AAA0 \cdots$  it is most likely that this offspring would recombine with the remaining  $2A$  particles and undergo another local sequence of reactions. And if in the meantime the  $3A$  in a row have either branched or undergone a  $3A \rightarrow 2A$  reaction, the remaining particles would not have the time to go very far. Since everything takes place essentially locally, the mean-field rate equation should be valid [18] yielding therefore  $\alpha=1/3$ .

To check this scenario I run simulations for the  $3A \rightarrow 4A$ ,  $3A \rightarrow \emptyset$  model, in which no such local sequence of reactions occur, since following the triplet annihilation the remaining single  $A$  can diffuse away at most.

The dynamical rules are very similar to those of the  $3A \rightarrow 4A$ ,  $3A \rightarrow \emptyset$  model. An elementary MCS consists of the following processes:

- (a)  $A\emptyset \leftrightarrow \emptyset A$  with probability  $D$ ,
- (b)  $3A \rightarrow \emptyset$  with probability  $p(1-D)$ ,
- (c)  $3A \rightarrow 4A$  with probability  $(1-p)(1-D)$ ,

such that the reactions were allowed on the left or right side

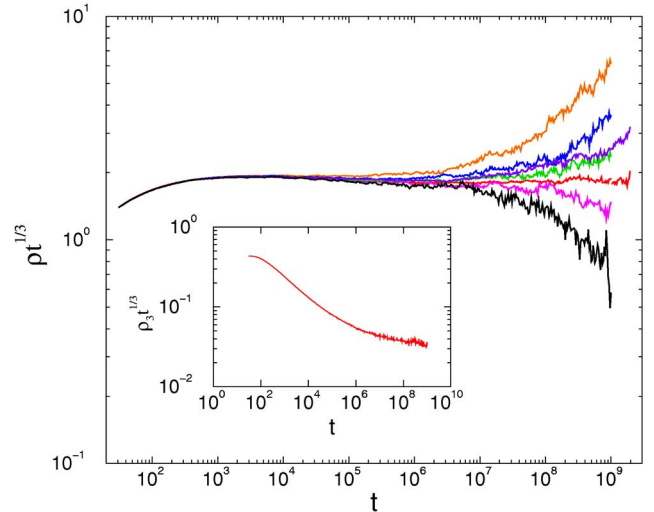


FIG. 4. (Color online) Density decay in the  $3A \rightarrow 4A$ ,  $3A \rightarrow \emptyset$  model at  $D=0.8$ . Different curves correspond to  $p=0.1185, 0.1187, 0.11875, 0.1188, 0.11886, 0.1189$ , and  $0.119$  (from top to bottom). The inset shows the decay of triplets for  $p=0.11886$ .

of the selected particle strings. Now the system size was  $4 \times L = 10^5$  with periodic boundary conditions and the density of particles, singlets and triplets are followed up to  $2 \times 10^9$  MCS from the random initial state. As Fig. 4 shows the time evolution of  $\rho(t)$  can be split into three parts (a) an initial slow regime ( $t < 3 \times 10^3$  MCS), (b) an intermediate faster then mean-field regime ( $3 \times 10^3 < t < 3 \times 10^6$  MCS), and (c) a mean-field regime for  $t > 3 \times 10^6$  MCS. One can see a level-off in the time evolution of  $\rho t^{1/3}$  for  $p=p_c=0.11887(2)$ . For this critical  $p$  value the density of triplets behaves in the same way in the long time limit ( $t \approx 3 \times 10^6$  MCS) corroborating the  $d_c=1$  result of the previous section.

Finally, the static exponent  $\beta$  was determined in the active phase in the neighborhood of the critical point ( $p_c=0.11887$ ). As Fig. 3 shows the local slopes (2) converge to the mean-field value again. By fitting with the form (4) one gets the following estimates:  $\beta=0.99(5)$ ,  $x=0.6(1)$ .

### IV. CONCLUSIONS

Large scale simulations for two different triplet models:  $3A \rightarrow 4A$ ,  $3A \rightarrow 2A$  and  $3A \rightarrow 4A$ ,  $3A \rightarrow \emptyset$  result in mean-field type of static and dynamic scaling behavior in one dimension. The simulations up to  $t=2 \times 10^9$  MCS do not support the scenario according to fluctuations are suppressed and which reactions take place locally hindering the PCPD type of critical behavior. Since the triplet density decays in the same way as the total density, which is typical at the upper critical dimension the  $d_c=1$  is concluded. Furthermore, the logarithmic correction to scaling is shown in the case of the static order parameter exponent. On the other hand, one can not see log corrections in the density decay, which may mean that these corrections are small or perhaps a next to the leading order correction term hinders it. Such a correction term was found in a very recent field the-

oretical analysis of the  $3A \rightarrow (\emptyset, A, 2A)$  models [19], which correspond to the dominant behavior in the inactive phase of the triplet model I studied.

The contradiction with the results of the Langevin equation analysis of a bosonic triplet system is unresolved. This may also mean that the two-species coupled model and the one-species model behave differently.

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