

Cluster mean-field study of the parity-conserving phase transition

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The phase transition of the branching and annihilating random walk with even offspring is studied by N -cluster mean-field approximations on one-dimensional lattices. By allowing the system to reach zero branching rate a phase transition can be seen for any $N \leq 12$. Coherent anomaly extrapolations applied for the series of approximations results in $\nu_{\perp} = 1.85(3)$ and $\beta = 0.96(2)$.

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I. INTRODUCTION

The study of nonequilibrium phase transition universality classes is one of the most fundamental tasks of statistical physics [1–6]. Such phenomena may appear in models of population, epidemics, catalysis, cooperative transport [1], and enzyme biology [7] for example. For a long time only the universality class of directed percolation (DP) [8] was known, but later it turned out that different classes may appear in other models (for a review see [3]). The most prominent example occurs in one-dimensional systems exhibiting Z_2 symmetrical absorbing states [9–13] and parity-conserving (PC)—explicit or underlying—branching and annihilating random walk with even offspring (BARWe) dynamics ($A \rightarrow 3A, 2A \rightarrow \emptyset$) of the dual variables (A) [14–17]. For a review see [18]. This class is also called the directed Ising, DP2, or generalized voter model class.

However, an understanding of these phenomena involving a satisfactory solution of the corresponding field theory is very rare. For BARWe models field theory failed to give quantitatively precise results in one dimension [17] because systematic epsilon expansion breaks down due to a second critical dimension at $d'_c = 4/3$ below $d_c = 2$. Very recently another field theory has been suggested and analyzed by numerical simulation of the Langevin equation for systems exhibiting Z_2 symmetric absorbing states [19]. Numerical approximations ranging from simulations [13,15,18,20,21] to series expansions [22], cluster mean-field approximations [11,21], and the empty interval method [23] established the values of critical exponents firmly.

Recently Zhong, ben-Avraham, and Muñoz (ZAM) [23] constructed a special parity-conserving (PC) reaction-diffusion model. By studying it up to pair approximations they claimed that cluster mean-field studies fail to reproduce the phase transition of the BARWe model if one considers clusters that are not large enough. Therefore one may arrive at the conclusion that the cluster mean-field and especially the site mean-field solutions break down generally in the case of PC class transitions. However, in that study the branching attempt probability (σ) was fixed to a finite value, so one should not expect to see the mean-field transition, which is known to occur at zero branching rate. In the present study we show that the cluster mean-field approximation can describe the mean-field transition qualitatively well even for small cluster sizes if we do not exclude the

neighborhood of the zero branching rate from the parameter space. These approximations are performed on one-dimensional clusters; therefore for large cluster sizes N one expects to see a convergence toward the PC class transition at $\sigma_c > 0$. We apply coherent anomaly extrapolations for the sequence of cluster mean-field results and give estimates for some exponents of the critical behavior in one dimension.

The interplay of diffusion and fluctuation has already been shown in many reaction-diffusion models (see, for example, [21,24–26]). Although the diffusion is unable to change the universal behavior it can affect the location of the transition and even more it can change the stability of a fixed point in the case of competing reactions [24–26]. To investigate the possible role of diffusion we also extend the parameter space by modifying the diffusion rate.

II. THE CLUSTER MEAN-FIELD METHOD

The generalized (cluster) mean-field (GMF) method is an extension of the usual mean-field calculation obtained by setting up master equations for n -point configuration probabilities of site variables $s_i \in \{A, \emptyset\}$,

$$\frac{\partial P_n(\{s_i\})}{\partial t} = f(P_n(\{s_i\})), \quad (1)$$

where the function f depends on the transition rules of $\{P_m\}$ “block probabilities” at time t .

At the level of N -point approximation the correlations are neglected for $n > N$, that is, $P_n(s_1, \dots, s_n)$ is expressed by using the Bayesian extension process [27–29],

$$P_n(s_1, \dots, s_n) = \frac{\prod_{j=0}^{j=n-N} P_N(s_{1+j}, \dots, s_{N+j})}{\prod_{j=1}^{j=n-N} P_{N-1}(s_{1+j}, \dots, s_{N-1+j})}. \quad (2)$$

In principle, $2^N - 1$ parameters are required to define the probability of all the N -point configurations. This number, however, is drastically reduced by the following conditions. In the stationary state the particle distribution is assumed to be symmetric with respect to translation and reflection. Furthermore, the block probability consistency results in

$$P_n(s_1, \dots, s_n) = \sum_{s_{n+1}} P_{n+1}(s_1, \dots, s_n, s_{n+1}),$$

$$P_n(s_1, \dots, s_n) = \sum_{s_0} P_{n+1}(s_0, s_1, \dots, s_n).$$

Here we apply the GMF method for one-dimensional, site restricted lattice versions of the BARWe. Taking into account the spatial symmetries in the case of the $N=10$ GMF approximation, one has to find the solution of equations of 528 independent variables. This has been achieved with the help of MATHEMATICA software. We required 20-digit accuracy in the results and arbitrary precision during the calculations.

It is well known that such approximations predict the phase structure qualitatively well in one dimension, provided N is large enough to take into account the relevant interaction terms. For example, $N > 1$ is needed to take into account particle diffusion terms, while $N > 2$ was found to be necessary in the case of binary production processes involving pair induced reactions [4,30]. The GMF is an efficient phase diagram exploration method and although it is set up for the $d=1$ lattice in previous cases it provided a qualitatively good phase diagram for higher dimensional, mean-field versions as well (see, for example, [31,25,32,33]).

III. THE ZAM MODEL

In [23] Zhong *et al.* defined a special, one-dimensional, parity-conserving lattice model in which each site is either empty or singly occupied. The state of the lattice is updated asynchronously by the following rules. An occupied site is chosen randomly and it is tried for diffusion, at rate Γ [probability $\Gamma/(\Gamma+\Omega)$], or branching, at rate Ω [probability $\Omega/(\Gamma+\Omega)$]; while the time is increased by $1/N$, where N is the number of occupied (active) sites. In a diffusion step the particle jumps to its randomly chosen nearest neighbor site. If the site is occupied both particles are annihilated with probability r . On the other hand the jump is rejected with probability $1-r$. The branching process involves the creation of two new particles around the neighborhood. If either or both neighboring sites is previously occupied the target site(s) becomes empty with probability r . Otherwise the lattice remains unaltered with probability $1-r$.

The site mean-field equation for the concentration c (probability of site occupancy) is

$$\frac{d}{dt}c = -2rc^2 + 2c(1-c)^2 - 2rc^3, \quad (3)$$

where $\Gamma=\Omega=1$ was taken; hence the branching probability is fixed to $1/2$. Similarly the $N=2$ pair mean-field approximation was solved and in both cases the system always evolves to an active phase with finite concentration c_s (see Fig. 1). These results were compared with those of the $r < 1$ rate model in one dimension, for which a PC class continuous phase transition is known at $r_c > 0$ [15]. The conclusion was drawn that cluster mean-field approximations of low orders fail to reproduce the phase diagram; the convergence is very slow and the calculations are complicated. However, it is also known that in the mean-field approximation—which is valid for $d > d_c = 2$ dimensions—the phase transition occurs at zero branching rate [17], so it is not surprising that by fixing $\Omega=1$ one does not see a phase transition in the corre-

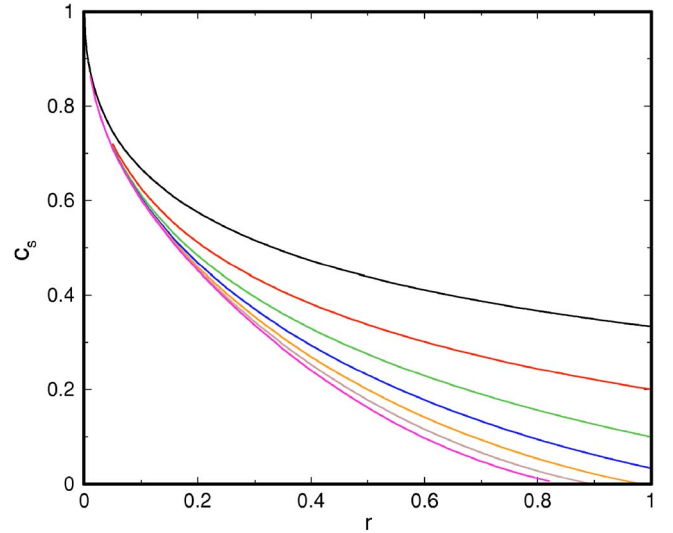


FIG. 1. (Color online) GMF results for the steady state concentration in the ZAM model for $N=1,2,\dots,7$ clusters (top to bottom).

sponding mean-field approximations. On the other hand, Zhong *et al.* found a phase transition for $0 < r_c < 1$ by the parity interval method—which also involves a mean-field-like approximation—set up for this one-dimensional model [23]. The authors acknowledged that it had been possible to see the phase transition in related PC class models for larger ($N > 2$) cluster sizes [11].

To clarify this we extended the cluster mean-field method for higher orders and for other versions of this BARWe model exhibiting a PC class transition.

We determined the steady state solutions of Eq. (1) taking into account Eqs. (2) and (3) and calculated the corresponding steady state densities $c_s(r)$ (see Fig. 1). Indeed higher levels of approximations ($N > 4$) of the ZAM model result in a phase transition with $r_c(N) \leq 1$ converging toward the simulation value [$r_c = 0.470(5)$].

IV. GMF RESULTS FOR THE MODIFIED ZAM MODEL

As we saw in the preceding section cluster mean-field approximations of the ZAM model give qualitatively good phase diagram for $N > 4$ and the steady state solutions converge to the Monte Carlo simulation results. However, going much further with the GMF study of the ZAM model is time consuming especially because the numerical root finding of Eq. (1) gets computationally demanding for large numbers of variables. On the other hand by modifying the ZAM model slightly in such a way that zero branching rate is allowed with the restriction $\sigma = 2\Omega/(\Gamma+\Omega) = 1-r$ (ZAMB model) one immediately finds the expected mean-field transition at $\sigma_c = 0$ for $N \geq 1$.

The site approximation equation for the concentration is

$$\frac{d}{dt}c = 2c[1 + c^2(r-1)^2 - r - c(2-r)], \quad (4)$$

exhibiting the steady state solution

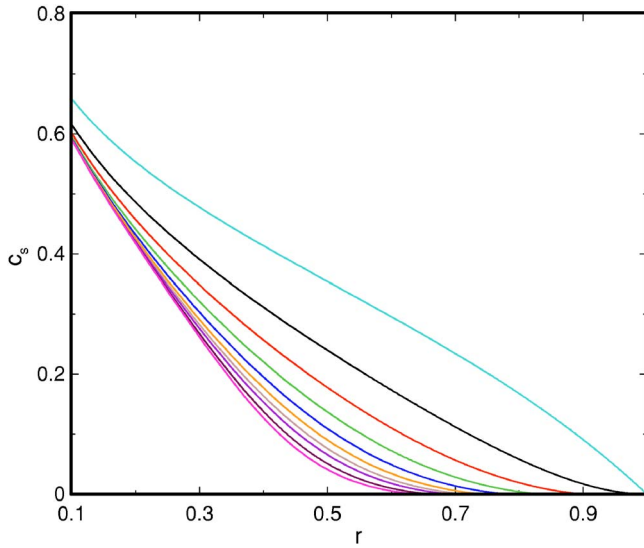


FIG. 2. (Color online) Steady state concentration GMF results for the ZAMB model for $N=1, 2, 3, 4, 5, 6, 7, 8, 10, 12$ clusters (top to bottom).

$$c_s = \frac{2 - r - \sqrt{r\sqrt{8 - 11r + 4r^2}}}{2(r-1)^2} \quad (5)$$

for $r < 1$. For $r=1$ Eq. (4) simplifies to

$$\frac{d}{dt}c = -2c^2, \quad (6)$$

resulting in $c \propto 1/t$ particle density decay in agreement with the mean-field expectations. The supercritical behavior in the active phase can be characterized by a $\beta=1$ leading order singularity for $r_c \leq 1$,

$$c_s \propto |r - r_c|^\beta, \quad (7)$$

and a $\beta'=2$ correction to scaling exponent defined as

$$c_s = a|r - r_c|^\beta + b|r - r_c|^{\beta'}. \quad (8)$$

The steady state solution has been determined for $N=1, 2, 3, 4, 5, 6, 7, 8, 10, 12$ (see Fig. 2). As one can see even the pair approximation gives $r_c(2)=1$, but for $N > 2$ the transition point starts shifting toward the true transition point $r_c < 1$ as expected in one dimension. One can also observe a concave shape of the curves corresponding to the corrections to scaling with exponent $\beta'=2$.

A. The effect of diffusion

In previous papers [11,34,31,24–26]) it was shown that the diffusion strength can cause relevant effects on the phase diagram of reaction-diffusion models when it competes with the reactions. This is reflected in the cluster mean-field approximations in such a way that stronger diffusion “washes out” fluctuations and causes a transition, which is more site mean-field-like, while higher N takes into account more fluctuations and hence opposes the effects of the diffusion. Here we investigated the effect of diffusion by lowering the hop-

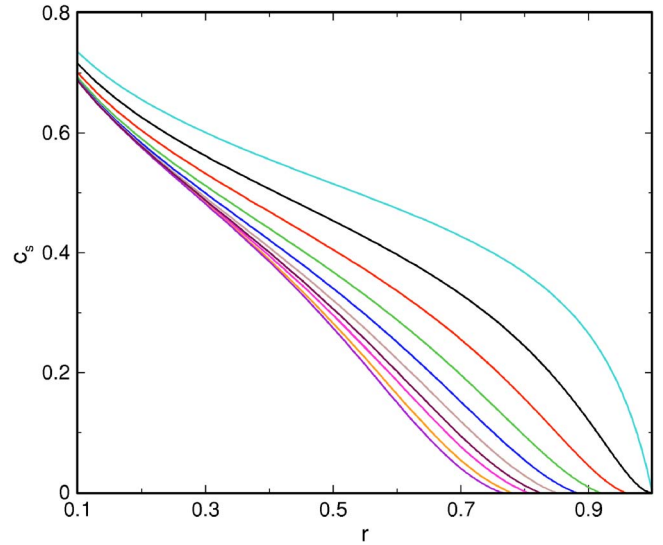


FIG. 3. (Color online) Steady state concentration GMF results for the ZAMB model for $D=0.2$ diffusion and $N=1, 2, 3, 4, 5, 6, 7, 8, 10, 12$ clusters (top to bottom)

ping probability of the ZAMB model to $D=2\Gamma/(\Gamma+\Omega)=0.2$. The steady state results (Fig. 3) show that the concentration curves arrive with higher slopes at the $c_s=0$ axis than in the case of $D=1$. This permits us to obtain $a(N)$ more precisely since the relative error of the amplitudes is smaller and the quadratic correction to scaling is weaker. As a consequence the numerical root finding is not so much affected by the basin of attraction of the absorbing state fixed point solution. Note that in the pair approximation the linear amplitudes $a(2)$ are zero.

V. SIMULATION RESULTS

By applying fitting with the expected scaling form

$$|r_c(N) - r_c|^{v_\perp} \propto 1/N \quad (9)$$

to the GMF data one can determine the location of the transition and v_\perp simultaneously. For $D=1$ this gives $r_c=0.402$, while for $D=0, 2$ $r_c=0.65$. However, to obtain better critical value estimates we used more precise r_c values in the fitting procedure, which can be deduced from simulations.

The simulations were performed on one-dimensional lattices of sizes $L=10^7$ with periodic boundary conditions. The runs were started from half filled lattices with randomly distributed particles. One elementary Monte Carlo step (MCS) consists of the following processes. A particle and a direction are selected randomly. If the nearest neighbour (NN) site in the selected direction is empty the particle moves to it (with probability D). If it is filled, both particles are removed (with probability r). The time—measured in MCSs—is updated by $1/n_p$, where n_p is the total particle number at time t . To perform the branching another particle is selected randomly (with probability $1-r$). Depending on the status of the two NNs (s_{i-1}, s_{i+1}) the following process may occur.

(a) If $s_{i-1}=s_{i+1}=\emptyset$, two new particles are created.

(b) If $s_{i-1}=s_{i+1}=A$ the two NN particles are removed with probability r .

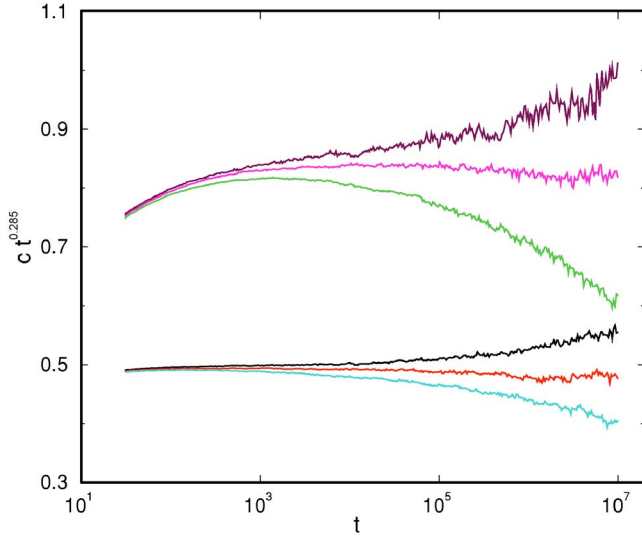


FIG. 4. (Color online) Particle density decay of the ZAMB model times the expected critical power law ($t^{0.285}$). Different curves correspond to $r=0.565, 0.562, 0.56$ and $D=0.2$, $r=0.408, 0.409, 0.41$ and $D=1$ (from top to bottom).

(c) If $s_{i-1} \neq s_{i+1}$ the NNs are swapped with probability r . The time (t) is updated by $1/n_p$ again. The simulations were followed up to $t=10^7$ MCS or until $n_p=0$ (absorbing state). The concentration of particles $c_s(t)$ times the expected density decay power law $1/c \propto t^{0.285}$ [18,20] is plotted on Fig. 4. One can read off $r_c=0.409(1)$ for $D=1$ and $r_c=0.562(1)$ for $D=0.2$. For $D=1$ this agrees well with the extrapolation results of Eq. (9) but for $D=0.2$ the deviation is not negligible.

VI. COHERENT ANOMALY EXTRAPOLATIONS

According to scaling theory the location of the critical point for sizes N [$r_c(N)$] scales (in the large N limit) as Eq. (9). Precise extrapolation can be obtained by applying the critical transition point values of simulation in the mentioned scaling form. The $r_c(N)$ for the N th level of approximations was determined by quadratic fitting for $c_s(N) < 0.002$. Figure 5 shows $r_c(N)$ as a function of $1/N$. The fit of the form (9) yields $1/\nu_{\perp}=0.54(1)$ for $D=1$ and $1/\nu_{\perp}=0.53(1)$ for $D=0.2$ (see Fig. 5). The value $\nu_{\perp}=1.85(3)$ agrees well with the value from the literature $\nu_{\perp}=1.84(6)$ [20] for this class.

We applied the coherent anomaly method (CAM) [35] for the N -cluster GMF results to extrapolate to the $N \rightarrow \infty$ behavior. This method has been proven to be successful for obtaining critical exponents of nonequilibrium absorbing phase transitions [11,21,36–38,32,39]. Earlier the GMF+CAM method was already used for analyzing the PC class transition of the nonequilibrium kinetic Ising model [11,21] up to cluster sizes $N \leq 6$. That study arrived at the rough estimate $\beta \approx 1$, which agrees with the series expansion result $\beta = 1.00(5)$ [40] and marginally the simulation results $\beta = 0.95(2)$ [18]. Now we apply this method for cluster sizes up to $N \leq 12$ and improve the GMF+CAM results [11,21] for a model exhibiting the PC class transition. According to the CAM the amplitudes $a(N)$ of the cluster mean-field singularities

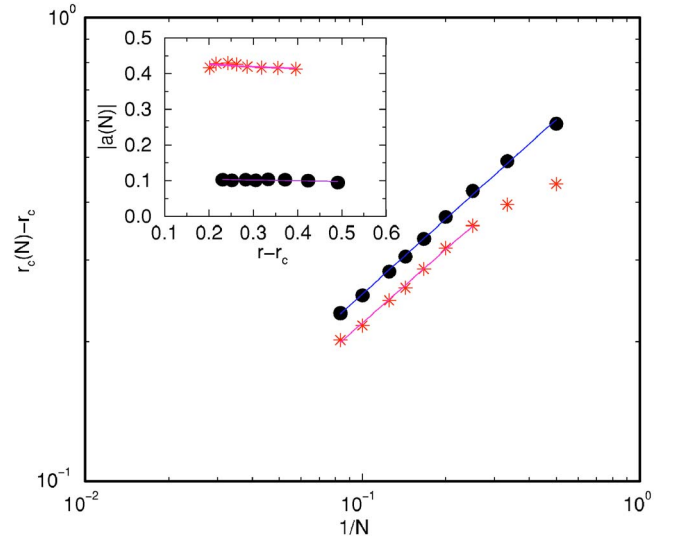


FIG. 5. (Color online) CAM extrapolation results for the critical point $r_c(N)$ ($2 \leq N \leq 12$). The inset shows $|a(N)|$ ($3 \leq N \leq 12$). Stars correspond to $D=1$, boxes to $D=0.2$. Numerical errors are smaller than the symbol sizes.

$$c_s(N) = |a(N)| |r_c(N) - r|^{\beta_{MF}} \quad (10)$$

scale in such a way

$$|a(N)| \propto |r_c(N) - r|^{\beta - \beta_{MF}} \quad (11)$$

that the exponent of the true singular behavior [Eq. (7)] can be estimated. The $a(N)$ amplitudes were determined by linear fitting to the local slopes of the $c_s(N)$ data in the neighborhood of $r_c(N)$. The amplitudes are shown in Table I and in the inset of Fig. 5. The fitting using the form Eq. (11) for $N > 2$ data [since $a(2)=0$] results in $\beta=0.92(5)$ for $D=1$ and $\beta=0.96(2)$ for $D=0.2$. The CAM for $D=1$ results in a bigger

TABLE I. Summary of results for the ZAMB model.

n	D			
	0.2		1	
	$r_c(N)$	$ a(N) $	$r_c(N)$	$ a(N) $
1	1	5	1	1
2	1	0	1	0
3	0.9575(2)	0.4124(4)	0.8997(2)	0.094(5)
4	0.9177(1)	0.4155(3)	0.8321(1)	0.100(8)
5	0.8802(4)	0.4167(9)	0.7805(1)	0.103(7)
6	0.8485(1)	0.4192(9)	0.7423(9)	0.104(7)
7	0.8235(1)	0.4254(3)	0.714(7)	0.100(12)
8	0.8044(1)	0.429(3)	0.691(13)	0.103(9)
10	0.7787(1)	0.427(2)	0.6608(1)	0.100(6)
12	0.7633(2)	0.416(2)	0.6394(1)	0.103(6)
r_c	0.562(1)		0.409(1)	
ν_{\perp}	1.88(3)			1.85(3)
β		0.96(2)		0.92(5)

numerical error than for $D=0.2$, because for $D=1$ the quadratic corrections to scaling are stronger and the $c_s(r)$ numerical solutions are affected by the attractive basin of the neighboring absorbing state fixed point. These values agree well with the simulation results $\beta=0.95(2)$ [18] and $\beta=0.94(6)$ [20] as well as with that of the parity interval method $\beta=0.92(2)$ [23].

VII. CONCLUSIONS

We showed that even low order GMF approximations can describe the phase transition of an even-offspringed BARWe model correctly if one allows appropriate parametrization. We applied GMF approximations for a one-dimensional site restricted lattice model. By allowing the model to reach the zero branching rate in the ZAM model we showed that the

site mean-field solution is in agreement with that of the field theory for this class [17]. Note that this kind of analysis resulted in similar steady state solutions in the case of another PC class model [11,21], although there the branching rate cannot be read off explicitly.

The GMF approximations were determined up to $N=12$ and convergence toward the simulation results were shown. Using scaling and CAM theory we obtained $\nu_{\perp}=1.85(3)$ and $\beta=0.96(2)$ critical value estimates matching the best precision available in the literature for the PC universality class.

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