Cluster mean-field study of the parity conserving phase transition

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

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 the directed percolation (DP) [8] has been 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 (BARWe) dynamics (\( A \to 3A, 2A \to \emptyset \)) of the dual variables (\( A \)) [14–17]. For a review see [18]. This class is also called as directed Ising, DP2 or generalized voter model class.

However understanding these phenomena involving a satisfying 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 brakes down due to a second critical dimension at \( d_c' = 4/3 \) below \( d_c = 2 \). Very recently an other 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 empty interval method [23] established the values of critical exponents firmly.

Recently Zhong et al. [23] constructed a special parity conserving reaction-diffusion model (hereafter we call it ZAM 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 which are not large enough. Therefore one may arrive to the conclusion that cluster mean-field and especially the site mean-field solution breaks down generally in case of PC class transitions. However in that study the branching attempt probability (\( \sigma \)) 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 approximations can describe the 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 towards 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 [21,27,29,30]). 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 case of competing reactions [27,29,30]). 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 by setting up master equations for \( n \)-point configuration probabilities of site variables \( s_i \in \{A, \emptyset\} \)

\[
\frac{\partial P_n(s_1)}{\partial t} = f(P_n(s_1))
\]

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

At the level of \( N \)-point approximation the correlations are neglected for \( n > N \), that is, \( P_n(s_1, ..., s_n) \) is expressed by using the Bayesian extension process [38–40],

\[
P_n(s_1, ..., s_n) = \frac{\prod_{j=1}^{N-n}s_{n+j}P_N(s_{1+j}, ..., s_{N+j})}{\prod_{j=1}^{N-n+1}s_{n+1+j}P_{N-1}(s_{1+j}, ..., s_{N-1+j})}.
\]

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 trans-
loration and reflection. Furthermore, the block probability
consistency results in:

\[ P_n(s_1, ..., s_n) = \sum_{s_{n+1}} P_{n+1}(s_1, ..., s_n, s_{n+1}) , \]

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

Here we apply GMF for one-dimensional, site re-
stricted lattice versions of BARWe. Taking into account
spatial the symmetries in case of the \( N = 10 \) GMF ap-
proximation 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 dur-
ing the calculations.

It is well known that such approximations predict the
phase structure qualitatively well in one dimension, pro-
vided \( N \) is large enough to take into account the rele-
vant interaction terms. For example \( N > 1 \) is needed to
take into account particle diffusion terms, while \( N > 2 \)
was found to be necessary in case of binary production
processes involving pair induced reactions [27,28]. The
GMF is an efficient phase diagram exploration method
and although it is set up for the \( d = 1 \) lattice in previ-
ous cases it provided qualitatively good phase diagram
for higher dimensional, mean-field versions as well (see
example [26,29,35,36]).

III. THE ZAM MODEL

In [23] Zhong et al. defined a special, one-dimensional,
parity conserving lattice model in which each site is ei-
ther empty or singly occupied. The state of the lattice is
updated asynchronously by the following rules: an occu-
pied site is chosen randomly and it is tried for diffusion,
with rate \( \Gamma \) (probability \( \Gamma / (\Gamma + \Omega) \)), or branch-
ing, at rate \( \Omega \) (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 ran-
domly chosen nearest neighbor site. If the site is occu-
pied both particles are annihilated with probability \( r \).
On the other hand the jump is rejected with probabil-
ity \( 1 - r \). 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) become 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 proba-

We determined the steady state solutions of Eq.(1) tak-
ing into account Eqs.(2,3) and calculated the correspond-
ing steady state densities \( c_s(r) \) (see Fig.1). Indeed higher
levels of approximations (\( N > 4 \)) of the ZAM model re-
sult in phase transition with \( r_c(N) \leq 1 \) converging to-
wards the simulations (\( r_c = 0.470(5) \)).
IV. GMF RESULTS FOR THE ZAMB 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 MC simulations. 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 number 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) one immediately finds the expected mean-field transition at $\sigma_c = 0$ for $N \geq 1$.

The site approximation equation for the concentration is

$$\frac{dc}{dt} = 2c \left(1 + c^2 (r - 1)^2 - r - c (2 - r)\right),$$  
(4)

exhibiting the steady state solution

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

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

$$\frac{dc}{dt} = -2c^2$$  
(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 $\beta = 1$ leading order singularity for $r_c \leq 1$

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

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

and

$$c_s = a|r - r_c|^\beta + b|r - r_c|^\beta'.$$  
(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 towards 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 $\beta' = 2$ exponent.

A. The effect of diffusion

In previous papers [11,25–27,29,30] 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, hence opposes the effects of the diffusion. Here we investigated the effect of diffusion by lowering the hopping 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 to the $c_s = 0$ axis than in 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 the

![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).](image1)

![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).](image2)
consequence the numerical root finding is not so much affected by 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

$$|r_c(N) - r_c| \nu_{\perp} \propto 1/N$$

(9)
to the GMF data one can determine the location of the transition and $\nu_{\perp}$ 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) in the selected direction was empty the particle moves to it (with probability $D$). If it was filled, both particles are removed (with probability $r$). The time – measured by MCS – 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 nn ($s_i-1, s_i+1$) 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 $r$.

c) If $s_i-1 \neq s_i+1$ the nn 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 critical 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 the function of $1/N$. The fit of 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.

![Graph](image1)

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).

![Graph](image2)

FIG. 5. (Color online) CAM extrapolation results for the critical point $r_c(N)$ ($2 \leq N \leq 12$). The insert 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.

We applied the coherent anomaly method (CAM) [31] for the $N$-cluster GMF results to extrapolate the $N \rightarrow \infty$ behavior. This method has been proven to be successful for obtaining critical exponents of nonequilibrium absorbing phase transitions [11,21,32-35,37]. Earlier the GMF+CAM method was already used for analyzing the PC class transition of the NEKIM [11,21]
up to \( N \leq 6 \) cluster sizes. That study arrived to the rough estimate \( \beta \simeq 1 \), which agrees with the the series expansion result \( \beta = 1.00(5) \) [41] and the simulation results marginally \( \beta = 0.95(2) \) [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 PC exhibiting PC class transition. According to CAM the amplitudes \( a(N) \) of the cluster mean-field singularities

\[
c_s(N) = |a(N)| r_c(N) - r \beta_{MF}
\]

scale in such a way

\[
|a(N)| \propto |r_c(N) - r\beta_{MF}|
\]

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 insert of Fig. 5. The fitting using 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 bigger 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], \( \beta = 0.94(6) \) [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-offsprung BARW model correctly if one allows appropriate parameterization. We applied GMF approximations for a one dimensional site restricted lattice model. By allowing 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 case of an other PC class model [11,21], although there the branching rate can’t be read-off explicitly.

The GMF approximations were determined up to \( N = 12 \) and convergence towards 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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