Dynamical mean-field approximations for a diffusive pair contact process

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Dynamical mean-field approximations are performed to study the phase transition of a pair contact process with diffusion in different spatial dimensions. The level of approximation is extended up to 18-site clusters for the one-dimensional model. The application of coherent anomaly method shows that the critical exponent does not depend on the strength of diffusion rate. The extension of the mean-field approximation to higher dimensions also suggests that the critical behavior may be described by a unique set of exponents.

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The study of nonequilibrium critical phenomena has received considerable attention but their understanding is far from complete. Even the simplest models can be theoretically challenging. A well-known example is the pair contact process model with diffusion (PCPD) [1]. Despite its intensive study there is no satisfying consensus about the accurate values of critical exponents (see Ref. [2] for a recent review and further references). Different methods and approximations were applied, such as Monte Carlo simulation (MC) [3, 4, 5, 6], dynamical mean-field approximation (DMF) [1, 7], density-matrix renormalization group study [1], and field-theoretic approach [8, 9]. Most of the studies have been devoted to the one-dimensional case but the published numerical results are partially contradictory. In addition to the simulation difficulties, a consistent field theory description of the model is still an unresolved issue [10]. Instead of summing all the raised proposals [2], we consider one of the suggestions that the value of critical exponent may depend on the strength of diffusion. This idea was inspired by different MC simulations [11, 12] and DMF approximations [13]. This latter approach, however, left some ambiguities for strong or very weak diffusion rate [14]. Subsequent simulations [15] revealed the concept of a novel universality class with a unique set of exponents. However exact calculation, albeit for a slightly different model, suggested the possibility of two transitions depending on the diffusion rate in higher spatial dimensions [16]. The primary purpose of this Brief Report to clarify the mentioned ambiguities of DMF approach by significantly improving the level of one-dimensional approximations and to extend the calculations to higher spatial dimensions.

The simplicity of PCPD model, especially in one dimension, makes possible to extend the DMF approximation to large-size clusters. Such a large number of approximations for the order parameter function enables the application of the coherent anomaly method (CAM) to derive quantitative prediction to the value of β exponent [17]. Another challenge is to develop the DMF approximation to higher spatial dimensions. Generally, such kind of calculation is expected to yield qualitatively correct results in high dimensions, therefore it can help us to clarify the raised question whether the values of critical exponents depend on the strength of diffusion rate.

The PCPD model [1, 14] is the extension of the pair-contact process model (PCP) [15] that belongs to the well-known DP universality class [16]. The PCPD model consists of a d-dimensional lattice, with periodic boundaries, where each site is either vacant or occupied by a single particle. The dynamical rules for updating the system are defined as follows. A randomly chosen pair of nearest-neighbor particles is annihilated with a probability \( p(1 - D) \). An additional particle is created around the given pair with probability \( (1 - p)(1 - D) \) if it is not forbidden by the exclusion principle. Furthermore individual particles are allowed to hop to the nearest-neighbor empty site with diffusion rate \( D \). This version is also called restricted PCPD model because the exclusion law prohibits double occupancy. In this model the order parameter is the concentration of pairs of particles \( \rho \) that becomes zero above a critical value of \( p \) when the system arrives to one of the two possible absorbing states [15].

The application of DMF approximation, which is a dynamical version of the cluster variation method, involves finding a hierarchy of evolution equations for the probability distributions of configurations within a cluster of \( n \) sites (for details, see e.g. Refs. [17, 18]). The calculation of transitions of cluster probabilities would generate infinite hierarchy of equations, since transitions in an \( n \)-site cluster may depend on sites outside the cluster. To avoid this the \( n \)-site approximation estimates \( m \)-site probabilities (for \( m > n \)) by using Bayesian extension process. This type of approximation has proved to be successful in the evaluation of phase diagram for many dif-
TABLE I: Results of \( n \)-site approximations for the one-dimensional model. The extrapolated values of \( p_c \) and the order parameter exponents \( \beta \) for different values of diffusion rate \( (D) \) are also given. Numbers in parentheses correspond to the uncertainty in the last digit.

| \( n \) \( \backslash \) \( D \) | 0.05 | 0.1 | 0.5 | 0.85 |
|---|---|---|---|---|
| \( p_c^n \) \( a_n \) | \( p_c^n \) \( a_n \) | \( p_c^n \) \( a_n \) | \( p_c^n \) \( a_n \) |
| 4 | 0.157167(1) 48.4(1) | 0.160964(1) 82.1(2) | 0.209694(2) 51.7(1) | 0.294937(1) 17.61(1) |
| 6 | 0.137271(1) 94.2(4) | 0.140885(1) 147.3(6) | 0.184175(4) 93.2(2) | 0.274965(2) 17.40(2) |
| 8 | 0.129264(2) 127.1(6) | 0.132484(4) 207.6(10) | 0.171820(6) 139.2(8) | 0.260674(6) 17.61(1) |
| 10 | 0.124488(5) 158.2(10) | 0.127542(4) 265.5(18) | 0.164401(6) 190.9(10) | 0.250095(8) 17.30(3) |
| 12 | 0.121299(7) 205.9(20) | 0.124240(10) 330.8(16) | 0.159422(8) 248.9(14) | 0.242122(12) 17.30(3) |
| 14 | 0.119015(7) 254.8(20) | 0.121799(10) 413.6(30) | 0.155843(10) 308.0(20) | 0.235710(16) 17.30(3) |
| 16 | 0.117303(3) 308.2(60) | 0.119963(10) 498.6(60) | 0.15309(4) 367.2(40) | 0.22676(12) 17.30(3) |
| 18 | 0.115964(4) 370.5(50) | 0.118411(11) 590.2(80) | 0.15053(10) 453.3(70) | 0.215710(16) 17.30(3) |

To eliminate these shortages now the approximation is extended up to \( n = 18 \) level. Naturally, for higher level approximations the equations can be only build and solved numerically \cite{25, 27}. The stationary distribution is attained via numerical integration when the sum of the absolute values of all time derivatives smaller than \( \epsilon \) (generally \( \epsilon = 10^{-8} \) is used). Increasing the level of approximation the necessary number of iterations to attain the steady-state configurations probabilities increases drastically. To demonstrate the speed of convergence for large \( n \), four-week running is necessary to get data at 18-point level. Despite the time consuming convergence during the iterations, the calculations are tractable even by a personal computer. Figure 1 illustrates the improvement of solutions as we increase the levels of approximation. Here the particle concentration functions \( \rho(p) \) are plotted for \( D = 0.1 \), which show linear decay around the transition point. The concentration of pairs can be displayed in a similar figure but \( u(p) \) decreases quadratically around \( p_c^n \) for \( n > 2 \).

The order-parameter exponent can be estimated from the mean-field data following the CAM approach developed by Suzuki \cite{13}. In the vicinity of the critical point the order parameter function can be fitted as \( u(p) \approx a_n (p_c^n - p)^{\beta_{MF}} \), where \( p_c^n \) denotes the value of the critical point at \( n \)-point level and \( p_c \) is the extrapolated value to the \( n \to \infty \) limit. As we mentioned \( \beta_{MF} = 2 \) is valid for all values of \( D \) if \( n > 2 \). Table II summarizes the results for the estimated transition points \( (p_c^n) \) and amplitudes \( (a_n) \) at different levels of approximation for various values of diffusion rate. (The starting point of fitting is determined when the corresponding particle concentration drops below 0.01.) According to the CAM analysis the amplitudes \( a_n \) scales as

\[
a_n \approx (p_c^n - p_c)^{\beta_{MF} - \beta_{MF}}.
\]

As a consequence, the log–log plot of the amplitudes vs. \( p_c^n - p_c \) yields an estimation for the \( \beta \) exponent. Figure 2

FIG. 2: CAM scaling of the critical mean-field coefficients for the order parameter at different values of the diffusion constant. The lines correspond to the \( \beta = 0.5 \) exponent. The results of \( n = 4, 6, 8, \ldots, 18 \)-point level of approximations are plotted from right to left.
shows these plots for different values of $D$. This figure indicates clearly that wrong value of $\beta$ could be deduced by this technique if the calculations are limited to small-size clusters. For large $n$, however, the power law fits of the corresponding amplitudes become possible. The deviation of $\alpha_n$ from an expected power law function is pronounced for large $D$ when $n$ are small. Although the convergence of $\alpha_n$ is obvious, still the uncertainty of the estimated $\beta$ value is close to 10%. The extrapolated values of $p_c$ and the $\beta$ exponents for different diffusion rates are also given in Table I. Within the mentioned uncertainty the same $\beta = 0.50(5)$ exponents can be fitted for all values of $D$ as displayed in Fig. 4. This $\beta$ value is comparable to some earlier published MC results [8, 9].

To end this section it is worth emphasizing the sensitivity of CAM on the levels of approximation. The comparison of Fig. 1 and Fig. 2 underlines the different behaviors of $p_c^n$ and $\alpha_n$ as a function of $n$. As an example, the approach of $\alpha_n$ to the power law function is significant if we increase $n$ from 8 to 18 for $D = 0.1$ but the location of the transition point changes less than 11%. Similar behavior was reported by a recent study [28] where the same model was investigated by DMF approximation up to $n = 13$ for $D = 0.5$.

In the light of a field-theoretic calculation [12] it is also interesting to extend our investigations to higher spatial dimensions ($d > 1$). The main question is whether two transitions exist as a function of diffusion rate, $D$. The lowest level that considers the value of $d$ is the pair approximation ($n = 2$). In spite of its failure in one dimension [11, 12], this approximation is expected to provide qualitatively correct behavior in higher dimensions. At this level the two independent variables are the particle concentration denoted by $\rho$ and the concentration of pairs $u$. The equations of their time evolution on a $d$ dimensional lattice can be written as

\begin{equation}
\dot{\rho} = -2(1-D)pu + (1-D)(1-p)\frac{u(\rho-u)}{\rho}
\end{equation}

\begin{equation}
\dot{u} = -(1-D)p\frac{u}{(\rho)2m} \sum_{k=0}^{2m} (k+1) \binom{2m}{k} (u)^k (\rho-u)^{2m-k} + (1-D)(1-p)\frac{u(\rho-u)}{\rho(1-\rho)^m} \sum_{k=0}^{m} (k+1) \binom{m}{k} (\rho-u)^k (1-2\rho+u)^{m-k} + D \frac{\rho-u}{\rho^m(1-\rho)^m} \sum_{f=0}^{m} \binom{m}{f} (\rho-u)^f (1-2\rho+u)^{m-f} \left( \sum_{b=0}^{m} \binom{m}{b} u^b (\rho-u)^{m-b} \right),
\end{equation}

where $m = 2d - 1$. By comparing these equations in case of $d = 1$ to the equations in Ref. [3], one can observe that a prefactor 2 is missing from the diffusion part of Eq. [3]. The slight difference can be explained as follows. When doing MC simulation an elementary diffusion process includes to choose a particle and a direction as well. Afterwards the jump is executed with probability $D$ if the target site is empty. Therefore, the probability to jump to a specified direction is equal to $D/(2d)$. The normalization is fulfilled by choosing the latter jumping rate.

Returning now to the above equations the solutions in the active phase are

\begin{equation}
\rho = \frac{1-p}{1-3p} u, \quad \text{where}
\end{equation}

\begin{equation}
u = \left(\frac{1-3p}{1-p}\right)^2 \frac{2m - (1-D)(2m 3p + 1 - p)}{2m - (1-D)(2m 3p + 1 - 3p)}
\end{equation}

As a consequence, the value of critical point is

\begin{equation}
p_c^{MF}(D, D) = \begin{cases}
\frac{1}{12d-3+D} & \text{if } 0 \leq D \leq \frac{1}{2(3d-1)} \\
\frac{1}{3} & \text{otherwise}
\end{cases}
\end{equation}

It means that, as in one dimension, two different regions can be detected at any finite values of $d$ as a function of $D$. Nevertheless, the region that characterizes the high-$D$ behavior, including $p_c = 1/3$, expands if we increase $d$ and in the infinite dimension limit the solution convergences to the solution of the one-site approximation. From this result one may conjecture that there is no different universality classes at low and high diffusion rate for the restricted PCPD in higher dimensions.

More convincing arguments can be achieved by performing DMF approximation for larger clusters in two dimensions. In the absence of diffusion ($D = 0$) the two-point approximation yields qualitatively incorrect result, since the particle concentration becomes zero at the transition point ($p_c^{2p} = 5/17 \approx 0.2941$). This is contrary to the MC result that revealed a finite ‘natural’ density, $\rho_{nat} = 0.1477$ at the transition point ($p_c = 0.2005$) for the PCP model [29]. The four-site approximation (on $2 \times 2$ clusters) yields a better estimation for the transition point ($p_c^{4p} = 0.2691(3)$), however, it also predicts zero particle concentration at the transition point. This latter failure is already diminished at nine-site ($3 \times 3$ clusters) approximation. As the inset of Fig. 3 shows, this level of approximation can already describe qualitatively well the behavior of
FIG. 3: The pair-density function of the two-dimensional model at 9-point level for $D = 0, 0.1, 0.5$ and 0.9 values (from left to right curves). The inset shows particle density at $D = 0$ for $n = 2, 4,$ and 9-point levels (from right to left curves).

the two-dimensional PCP model: it gives $\rho_{nat} = 0.1197(2)$ at $p_{cr}^2 = 0.22607(3)$. The reason why the 9-point level gives a qualitatively different result may be explained by the fact that the $3 \times 3$ cluster size is the smallest cluster that covers all the elementary processes. (For example, a particle creation at the ends of an occupied pair “requires” a minimum size of 3 in one direction.) Similar qualitative improvement of the results have already been observed in a two-offspring branching annihilating random walk model [30]. In the latter one-dimensional model at least 5-point level of approximation was necessary for the correct description. The success of 9-point level of approximation also means that the smallest cluster that may give correct description of our PCPD model in three dimensions consists $3 \times 3 \times 3 = 27$ lattice points. This level is not obtainable presently. Returning to the two-dimensional case, the 9-point approximation does not predict qualitatively different behavior for low and high diffusion rate. Figure 4 demonstrates that the value of critical point increases with $D$ ($p_{cr}^2(D = 0.1) = 0.2607(5), p_{cr}^2(D = 0.9) = 0.3315(5)$) while the order parameter function does not differ qualitatively for $D = 0.1$ and $D = 0.9$. This result also supports the single universality class conjecture.

To summarize, DMF approximation is extended to large-cluster levels to study the critical behavior of the one-dimensional restricted PCPD model. We find that the ambiguity of CAM approach for weak and strong $D$ can be resolved by increasing the level of approximation. The approximation suggests uniform $\beta$ exponent for all values of $D$ within the uncertainty of the estimations. This $\beta = 0.50(5)$ value is comparable with some published MC results and supports that the model leaves the DP universality class and described by an exponent that also differs from the PC class. The approximations in higher dimensions also support the conjecture that the PCPD model can be described by a single universality class that is independently from the rate of diffusion.

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