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Double domain structure of the pair contact process with diffusion

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We investigate the domain structure of the pair contact process with diffusion (PCPD). PCPD is a stochastic reaction-diffusion model which evolves by the competition of two binary reactions, $2A \rightarrow 3A$ and $2A \rightarrow 0$. In addition, each particle diffuses isotropically, which leads to the bidirectional coupling between solitary particles and pairs. The spreading domain formed from localized activities in vacuum consists of two regions: The coupled region of size R_p where pairs and solitary particles coexist and the uncoupled region of size R_U where only solitary particles exist, respectively. The size of the whole domain R is given as $R=R_p+R_U$. At criticality, R_p and R_U scale as $R_p \sim t^{1/Z_p}$ and $R_U \sim t^{1/Z_U}$ with $Z_U > Z_p$. We estimate $Z_p=1.61(1)$ and $Z_U=1.768(8)$. Hence the correction to the scaling of R, $Q=R_U/R_p$ slowly decays extremely, which makes it practically impossible to identify the asymptotic scaling behavior of R. The double domain structure is another reason for the extremely slow approach to the asymptotic scaling regime of PCPD.

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Nonequilibrium absorbing phase transitions (APT's) from fluctuating active states into absorbing states in which the system is trapped forever have been a field of growing interest during past decades [1–3]. Recent theoretical and numerical studies show that APT's exhibit universality and it can be classified according to conservation laws, dimensionality of systems and symmetries of absorbing states [1–3]. However only a few universality classes have been identified so far. Directed percolation (DP) [2–5] and parity conserving (PC) [6–12] class are well studied classes among others. DP class includes systems with no special attributes except the time reversal symmetry, so that most systems studied so far belong to this class.

As a research direction to search for further unknown universality classes, coupled systems have been studied recently [8,13–25]. A coupled system is a multi-species system in which each species is coupled to the others in certain ways such as bidirectional and unidirectional coupling in linear or quadratic ways. However the coupled systems do not always exhibit new critical behavior. For bidirectionally coupled systems, the critical behavior depends on the manner of the coupling. For instance, quadratically coupled DP systems still belong to DP class despite their complex behavior [13]. However, linearly coupled systems belonging to DP or PC class exhibit mean-field or nontrivial critical behavior [8,14–17]. Linearly and unidirectionally coupled systems exhibit new critical behavior at multicritical point where all subsystems are critical [18–25].

Among single species systems, pair contact process with diffusion (PCPD) can be regarded as a two species system. PCPD has been extensively studied during past years due to its nontrivial critical behavior (see [26] for review). However, in spite of extensive theoretical and numerical studies, the critical behavior is not clearly uncovered yet. PCPD is a stochastic reaction-diffusion model, which evolves by the competition of two processes, fission ($2A \rightarrow 3A$) and annihilation ($2A \rightarrow \emptyset$). In addition, each particle performs isotropic diffusion. Without diffusion, the model is so-called pair contact process (PCP) belonging to DP class [27]. Since the reactions involve pairs, diffusing solitary particles are not engaged in the binary reactions. However when two solitary particles form a pair, the reactions take place. On the other hand, solitary particles are created from pairs by diffusion. Hence, PCPD can be regarded as a bidirectionally coupled two species system in which the order of the coupling is linear in the direction from pairs to solitary particles and quadratic in the opposite direction. This observation leads to the cyclically coupled DP and pair annihilation which exhibits the similar type of critical behavior to that of PCPD [28].

In this paper, we investigate the domain structure of PCPD. When a spreading domain is formed from localized initial activities, the quadratic coupling from solitary particles to pairs allows the pair-free region in which only solitary particles are present. We call the pair-free region so-called *uncoupled* region. On the other hand, the linear coupling from pairs to solitary particles results in the so-called *coupled* region in which pairs and solitary particles coexist. The pair-free region encloses the coupled region as shown in Fig. 1. Hence the spreading domain is divided into two regions, coupled and uncoupled region. This kind of double domain structure was found in unidirectionally coupled two level hierarchies [24,25]. As shown in previous studies on unidirectionally coupled systems [21–25], the measurements of critical exponents are very difficult due to long-time drift of the exponents. The one reason of the drift is the generic feature of the unidirectional coupling [21,22], the other is the double domain structure [24,25]. In measuring critical exponents, one can overcome the latter effect by measuring quantities in each region separately.

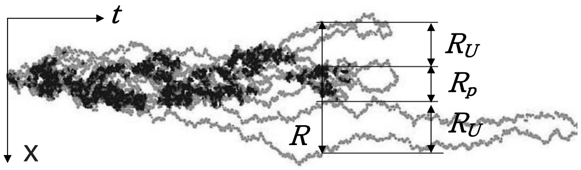

FIG. 1. Double domain structure of PCPD. The region with size R_p is the coupled region in which pairs (black) and solitary particles (gray) coexist. The region with size R_U is the uncoupled region in which only solitary particles exist.

As in unidirectionally coupled systems, it is expected that the double domain structure of PCPD also makes it difficult to identify the critical spreading behavior precisely. The aim of this paper is to investigate the effect of the double domain structure on the critical spreading of PCPD and to estimate critical exponents more precisely. We consider the PCPD of Ref. [29]. In this model, a randomly selected particle attempts to hop to one of the nearest neighbor sites with an equal probability. If the target site is empty, the attempt is accepted. However if the target site is occupied, (i) two particles annihilate with probability p or (ii) the hopping attempt is rejected and the pair (the chosen particle and one at the target site) tries to create a particle at the randomly chosen nearest neighbor site of the pair. When the target site is occupied, the branching attempt is rejected. The critical point of this model is $p_c=0.133\,519(3)$ in one dimension [29].

PCPD has three sectors in configuration spaces according to the existence of pairs (P) and solitary particles (S). The one is the configurations in which both pairs and solitary particles are present (*PS*-ensemble). We call configurations with at least one pair (two solitary particles) *P*-ensemble (*S*-ensemble). In *P*-ensemble (*S*-ensemble), solitary particles (pairs) may be present or not. The *P*-ensemble is the reactive subspace of Ref. [30]. A conventional ensemble includes configurations with at least two particles which can be either two solitary particles or one pair. We call the conventional ensemble *All*-ensemble. Since solitary particles are effectively linearly coupled to pairs, the existence of pairs implies the existence of solitary particles. Hence *PS*-ensemble should coincide with *P*-ensemble asymptotically. However, solitary particles transform into pairs by collisions, the coupling in this direction is quadratic. Hence the existence of solitary particles does not always guarantee the presence of pairs due to the long life time of solitary particles. So *S*-ensemble coincide with *All*-ensemble. As a result, there are two distinct ensembles in PCPD.

We define the size of each domain as follows (see Fig. 1). The size of the whole domain at time t $[R(t)]$ is defined as the distance between the leftmost and the rightmost particle. When both pairs and solitary particles exist simultaneously, we can define the size of the coupled region $[R_C(t)]$ and the size of the uncoupled region $[R_U(t)]$. Since solitary particles are linearly coupled to pairs, we define the size of the coupled region $[R_C(t)]$ as the spreading distance of pairs (R_p) defined as the distance between the leftmost and the rightmost pair. Then, $R_U(t)$ is given as $R_U=R-R_p$. Hence, we have three different lengths, R, R_p, and R_U in PCPD. To take into account the three length scales at the same time, one should use *PS*-ensemble in which only two lengths, R_p and R_U are the fundamental length scales of PCPD due to $R=R_p+R_U$.

At $p_c=0.133\,519$, we perform defect Monte Carlo simulations with a pair on a one-dimensional empty lattice. We run simulations up to $t=10^7$ time steps using 3.6×10^6 independent runs. We measure the squared sizes, R^2, R_p^2, and R_U^2 for surviving *PS*-ensemble. The PCPD has two absorbing states, vacuum and states with one diffusing solitary particle. Hence, we stop the simulations when the total number of particles N is less than 2. At the criticality, the squared sizes scale as $R^2\sim t^{2/Z}$, $R_p^2\sim t^{2/Z_p}$ and $R_U^2\sim t^{2/Z_U}$. Figure 2 shows the scaling plots of the squared sizes, $R_x^2/t^{2/Z_x}$. We obtain the best scaling plot with $Z=1.663(5)$, $Z_p=1.61(1)$, and $Z_U=1.768(8)$, respectively. The errors of our estimates should be larger due to the error of p_c. Within the numerical errors at the criticality, our estimate of Z agrees with the previous studies [26], especially $Z=1.70(5)$ [9]. Since $Z_U>Z_p$, the total spreading distance $R(=R_p+R_U)$ should scale as $R\sim t^{1/Z_p}$, and R_U plays the role of the correction to the scaling as in unidirectionally coupled systems. Hence, we conclude $Z=Z_p=1.61(1)$ which is the smallest value among the estimates of previous studies [26]. For reference, we also measure R^2 using *All*-ensemble. The difference of *All*-ensemble from *PS*-ensemble or *P*-ensemble is that *All*-ensemble includes configurations without pairs. Since solitary particles spread diffusively, it is expected that R averaged over *All*-ensemble scales differently from that of *PS*-ensemble. From the scaling plot of $R^2/t^{2/Z}$, we estimate $Z=1.676(3)$ for *All*-ensemble which is larger than that of *PS*-ensemble (not shown). The slow spreading of the whole domain in *All*-ensemble results from the diffusive motions of solitary particles in configuration without pairs.

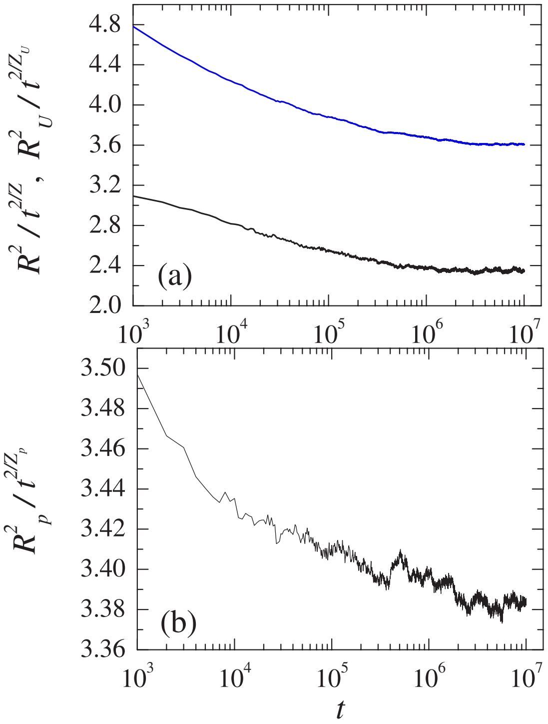

FIG. 2. (Color online) Scaling plots of various sizes. (a) The scaling plot of R^2 (lower curve) and R_U^2 (upper curve) with $Z=1.663$ and $Z_U=1.768$. (b) The scaling plot of R_p^2 with $Z_p=1.61$.

Since R scales as $R=R_p(1+R_U/R_p)$, the correction to the R is $Q=R_U/R_p$ which decays as $Q\sim t^{-\phi}$ with $\phi=(Z_U-Z_p)/Z_pZ_U$. To see how the correction decays slowly in time, we plot Q in Fig. 3. When $Q\ll1$, the correction is negligible. However, as shown in the inset, Q is still comparable to one even at $t=10^7$. We obtain the best scaling plot of Qt^{ϕ} with $\phi=0.054(4)$. As Q decays with very small ϕ, it is practically impossible to reach the asymptotic scaling regime of $R\sim R_p$. As a result, one should take the double domain struc-

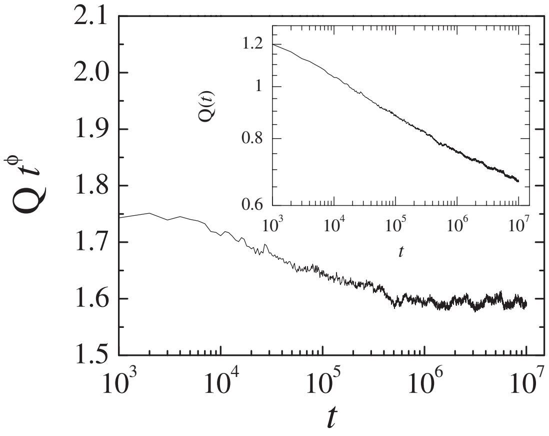

FIG. 3. Scaling plot of the ratio $Q=R_U/R_p$. The main plot shows Qt^{ϕ} with $\phi=0.054$. The inset shows the double logarithmic plot of $Q(t)$.

ture into account for the more precise measurement of the dynamic exponent Z.

In addition to the sizes, we also measure the number of pairs (N_p) and of solitary particles (N_s) averaged over all samples, and the survival probability of *PS*-ensemble (P_{ps}) and *All*-ensemble (P_{all}). As solitary particles are linearly coupled to pairs, N_s is proportional to N_p. At criticality, N_p scales as $N_p\sim t^{\eta}$. Figure 4 shows the scaling plot N_p/t^{η}. We obtain the best scaling plot with $\eta=0.275(5)$. The inset show the ratio of N_s/N_p, which converges to one as expected. $P_{ps}(t)$ and $P_{all}(t)$ decay in power law as $P_{ps}\sim t^{-\delta'_{ps}}$and $P_{all}\sim t^{-\delta'_a}$ at the criticality. Figure 5 shows the scaling plots of $P_x t^{\delta'_x}$ and the double logarithmic plots of P_{ps} and P_{all}. With $\delta'_{ps}=\delta'_a=0.130(3)$, we obtain the best scaling plots. The system escapes from the nonreactive sector in which only diffusing solitary particles are present via pair annihilations of solitary particles. As a naive argument for the equality of $\delta'_{ps}=\delta'_a$, the escaping probability from non-reactive sector within time τ may scale as $\tau^{-3/2}$ which is the death probability of two diffusing particles undergoing the reaction $S+S\to 0$ within τ. Hence, the contribution of non-reactive sector to P_{all} is negligible due to the fast escaping probability, which leads to the same scaling behavior of P_{all} as P_p.

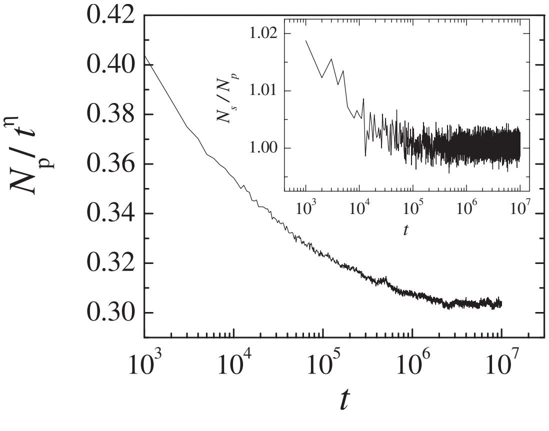

FIG. 4. Scaling plot of N_p. The main plot shows N_p/t^{η} with $\eta=0.275$. The inset shows the semilogarithmic plot of the ratio N_s/N_p.

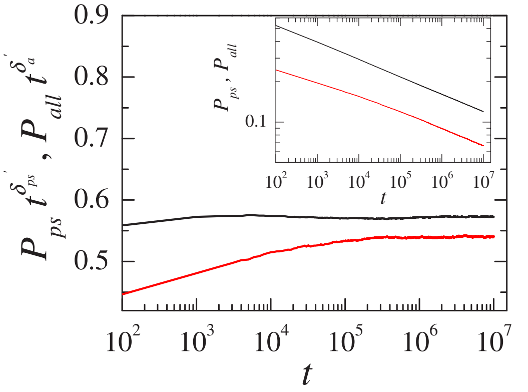

FIG. 5. (Color online) Scaling plot of P_{ps} and P_{all}. The main plot shows the scaling plot of $P_{ps}t^{\delta'_{ps}}$ (lower curve) and $P_{all}t^{\delta'_a}$ (upper curve) with $\delta'_{ps}=\delta'_a=0.13$. We add a constant −0.4 to the scaling plot of P_{all} for a better presentation. The inset shows the double logarithmic plots.

In summary, we investigate the domain structure of PCPD, and numerically confirm the existence of the double domain structure. This double domain structure comes from the linear and quadratic bidirectional couplings. The structure intrinsically makes the serious correction to the scaling of the critical spreading of a domain.

Starting with a pair, a domain grows and spreads in vacuum via fission ($2A\to 3A$) and spontaneous annihilation of pairs ($2A\to 0$) in PCPD. In addition to the binary reactions, each particle diffuses isotropically, which leads to the bidirectional coupling between solitary particles and pairs. The coupling from pairs to solitary particles is linear, while the opposite coupling is quadratic. The difference of the coupling ways results in the double domain structure of the whole domain, the coupled and the uncoupled region respectively. As a result, the size of the whole domain (R) is given as the sum of the size of the coupled region (R_p) and of the uncoupled region (R_U). We numerically find that R_p and R_U scale as $R_p\sim t^{1/Z_p}$ and $R_U\sim t^{1/Z_U}$ with $Z_U>Z_C$ at criticality. Hence, R should asymptotically scale as $R\sim t^{1/Z}$ with $Z=Z_p$ and R_U plays the role of the correction to the scaling. However, the direct measurement of R leads to the underestimate of the asymptotic value of Z because the correction $Q=R_U/R_p$ decays with very small exponent. Since it is practically impossible to reach the asymptotic scaling region of $R\sim t^{1/Z_p}$, it is important to take the domain structure into account in simulations for more precise estimate of the dynamic exponent Z of PCPD.

We classify particle configurations into four ensembles, which are finally reduced to two distinct ensembles, *P*-ensemble and *All*-ensemble respectively. *All*-ensemble includes configurations without pairs, while *P*-ensemble does not. The survival probabilities of two ensembles decay with the same exponent. However, the whole domain appears to spread more slowly in *All*-ensemble than in *P*-ensemble due to the diffusive motions of solitary particles in configurations without pairs. Hence, in addition to the domain structure, the diffusive motions of solitary particles in *All*-ensemble raise another correction to the scaling of the total spreading distance R which does not appear in P-ensemble.

As the linear-quadratic bidirectional coupling is the common feature of various PCPD studied so far, the double domain structure should appear in other PCPD variants. Among PCPD variants, we investigate the domain structure of the bosonic PCPD with soft constraint of Ref. [9]. For this model, we also confirm the existence of the double domain structure and the critical spreading behavior similar to that of PCPD studied in this paper. Hence, the double domain structure is a common feature of PCPD variants.

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