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Monte Carlo simulations of the smeared phase transition in a contact process with extended defects

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Abstract

We study the nonequilibrium phase transition in a contact process with extended quenched defects by means of Monte Carlo simulations. We find that the spatial disorder correlations dramatically increase the effects of the impurities. As a result, the sharp phase transition is completely destroyed by smearing. This is caused by effects similar to but stronger than the usual Griffiths phenomena, namely, rare strongly coupled spatial regions can undergo the phase transition independently from the bulk system. We determine both the stationary density in the vicinity of the smeared transition and its time evolution, and compare the simulation results to a recent theory based on extremal statistics.

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1. Introduction

Rare regions are an important, if intricate, aspect of systems with impurities and defects. In recent years, their influence on phase transitions and critical phenomena has reattracted considerable attention. Rare region effects were first studied in the context of classical equilibrium phase transitions. Griffiths [1] showed that they lead to a singular free energy in an entire parameter region in the vicinity of the phase transition, now known as the Griffiths region. However, in classical systems with uncorrelated disorder, this Griffiths singularity in the free energy is an essential one and thus very weak and probably unobservable in experiment. Disorder correlations generically increase the effects of impurities. Therefore, stronger rare region effects have been found in classical systems with extended defects and in random quantum systems (where the correlations are in the imaginary time direction). In the random transverse field Ising model [2] or, equivalently, the classical McCoy–Wu model [3], the Griffiths singularity takes a power law form, accompanied by a diverging magnetic susceptibility in the Griffiths region. Very recently, it has been found that some phase transitions can even be completely destroyed by smearing when the rare regions order independently from the bulk system. This happens, e.g., in a classical Ising magnet with planar defects [4] and in itinerant quantum ferromagnets [5].

In this paper, we investigate the effects of rare regions on *nonequilibrium* phase transitions with quenched spatial disorder. We concentrate on the prominent class of absorbing state phase transitions which separate active, fluctuating states from inactive, absorbing states where fluctuations cease entirely [6–9]. The generic universality class for absorbing state transitions is directed percolation (DP) [10]. According to a conjecture by Janssen and Grassberger [11], all absorbing state transitions with a scalar-order parameter, short-range interactions and no extra symmetries or conservation laws belong to this class. Examples include the transitions in the contact process [12], catalytic reactions [13], interface growth [14], or turbulence [15].

The effects of *uncorrelated* spatial disorder, i.e., point-like defects, on the DP transition have been studied in some detail in the past. According to the Harris criterion [16, 17], the DP universality class is unstable against spatial disorder, because the (spatial) correlation length exponent $\nu_\perp$ violates the inequality $\nu_\perp > 2/d$ for all spatial dimensionalities $d < 4$. Indeed, in the corresponding field theory, spatial disorder leads to runaway flow of the renormalization group (RG) equations [18], destroying the DP behaviour. Several other studies [19–22] agreed on the instability of DP against spatial disorder, but a consistent picture has been slow to evolve. Recently, Hooyberghs *et al* applied the Hamiltonian formalism [23] to the contact process with spatial disorder [24]. Using a version of the Ma–Dasgupta–Hu strong-disorder RG [25] these authors showed that the transition (at least for sufficiently strong disorder) is controlled by an exotic infinite-randomness fixed point with activated rather than the usual power-law scaling.

Very recently, it has been suggested [26] that extended spatial defects like dislocations, disordered layers, or grain boundaries can have an even more dramatic effect on nonequilibrium phase transitions in the DP universality class. Rare region effects similar to but stronger than the usual Griffiths phenomena [1, 17] actually destroy the sharp transition by smearing. This happens because rare strongly coupled spatial regions can undergo the transition independently from the bulk system. Based on an extremal statistics approach it has been predicted [26] that the spatial density distribution in the tail of the smeared transition is very inhomogeneous, with the average stationary density and the survival probability depending exponentially on the control parameter.

In this paper we present results of extensive Monte Carlo simulations of a two-dimensional contact process with linear spatial defects which provide numerical evidence for this smearing scenario in a realistic model with short-range couplings. The paper is organized as follows. In section 2, we introduce the model and briefly summarize the results of the extremal statistics theory for the smeared phase transition. In section 3 we present our simulation method and the numerical results together with a comparison to the theoretical predictions. We conclude in section 4 by discussing the importance of our results and their generality.

2. Theory

2.1. Contact process with extended impurities

The contact process [12] is a prototypical system in the directed percolation universality class. It can be interpreted, e.g., as a model for the spreading of a disease. The contact process is defined on a d-dimensional hypercubic lattice. Each lattice site $\mathbf{r}$ can be active (occupied by a particle) or inactive (empty). During the time evolution, active sites can infect their neighbours or they can spontaneously become inactive. Specifically, particles are created at empty sites at a rate $\lambda n/(2d)$ where n is the number of active nearest-neighbour sites and the 'birth rate' λ is the control parameter. Particles are annihilated at unit rate. For small birth rate λ, annihilation dominates, and the absorbing state without any particles is the only steady state (inactive phase). For large birth rate λ, there is a steady state with finite particle density (active phase). The two phases are separated by a nonequilibrium phase transition in the DP universality class at $\lambda = \lambda_c^0$.

Quenched spatial disorder can be introduced by making the birth rate λ a random function of the lattice site. Point-like defects are described by spatially uncorrelated disorder. We are interested in the case of extended defects which can be described by disorder perfectly correlated in d_{cor} dimensions, but uncorrelated in the remaining $d_r = d - d_{\text{cor}}$ dimensions. Here $d_{\text{cor}} = 1$ and 2 corresponds to linear and planar defects, respectively. Thus, λ is a function of $\mathbf{r}_r$ which is the projection of the position vector $\mathbf{r}$ on the uncorrelated directions. For definiteness, we assume that the birthrate values $\lambda(\mathbf{r}_r)$ are drawn from a binary probability distribution

$$P[\lambda(\mathbf{r}_r)] = (1-p)\delta[\lambda(\mathbf{r}_r) - \lambda] + p\delta[\lambda(\mathbf{r}_r) - c\lambda] \tag{1}$$

where p and c are constants between 0 and 1. In other words, there are extended impurities of spatial density p where the birth rate λ is reduced by a factor c.

2.2. Smeared phase transition

In this subsection, we briefly summarize the arguments leading to the smearing of the phase transition and the predictions of the extremal statistics theory [26] to the extent necessary for the comparison with the Monte Carlo results.

In analogy to the Griffiths phenomena [1, 17], there is a small but finite probability w for finding a large spatial region of linear size L_r (in the uncorrelated directions) devoid of impurities. Up to pre-exponential factors, this probability is given by

$$w \sim \exp\left(-\tilde{p} L_r^{d_r}\right) \tag{2}$$

with $\tilde{p} = -\ln(1-p)$. These rare regions can be locally in the active phase, even if the bulk system is still in the inactive phase. Since the impurities in our system are extended, each rare region is infinite in d_{cor} dimensions but finite in the remaining d_r dimensions. This is a crucial difference to systems with uncorrelated disorder, where the rare regions are finite. In our system, each rare region can therefore undergo a true phase transition *independently* of the rest of the system at some $\lambda_c(L_r) > \lambda_c^0$. According to finite-size scaling [27],

$$\lambda_c(L_r) - \lambda_c^0 = A L_r^{-\phi}, \tag{3}$$

where ϕ is the clean (d-dimensional) finite-size scaling shift exponent and A is the amplitude for the crossover from a d-dimensional bulk system to a 'slab' infinite in d_{cor} dimensions but finite in d_r dimensions. If the total dimensionality $d = d_{\text{cor}} + d_r < 4$, hyperscaling is valid, and $\phi = 1/\nu_\perp$ which we assume from now on.

The resulting global phase transition is very different from a conventional continuous phase transition, where a nonzero-order parameter develops as a collective effect of the entire system, accompanied by a diverging correlation length in all directions. In contrast, in our system, the order parameter develops very inhomogeneously in space with different parts of the system (i.e., different $\mathbf{r}_r$ regions) ordering independently at different λ. Correspondingly, the correlation length in the uncorrelated directions remains finite across the transition. This defines a smeared transition.

In order to determine the global system properties in the vicinity of the smeared transition, we combine (2) and (3) to obtain the probability for finding a rare region which becomes active at λ_c as

$$w(\lambda_c) \sim \exp\left(-B\left(\lambda_c - \lambda_c^0\right)^{-d_r \nu_\perp}\right) \tag{4}$$

for $\lambda_c - \lambda_c^0 \to 0+$. Here, $B = \tilde{p} A^{d_r \nu_\perp}$.

The total density ρ (the total number of active sites) at a certain λ is obtained by summing over all active rare regions, i.e., all regions with $\lambda > \lambda_c$. Since the functional dependence on λ of the density on any given active island is of power-law type it does not enter the leading exponentials but only the pre-exponential factors. Thus, the stationary density develops an exponential tail,

$$\rho_{\mathrm{st}}(\lambda) \sim \exp\left(-B\left(\lambda - \lambda_c^0\right)^{-d_r \nu_\perp}\right), \tag{5}$$

for all birth rates λ above the clean critical point λ_c^0. Analogous arguments can be made for the survival probability $P(\lambda)$ of a single seed site. If the seed site is on an active rare region it will survive with a probability that depends on λ via a power law. If it is not on an active rare region, the seed will die. To exponential accuracy the survival probability is thus also given by (5). The local spatial density distribution in the tail of the smeared transition is very inhomogeneous. On active rare regions, the density is of the same order of magnitude as in the clean system. Away from these regions it is exponentially small.

We now turn to the dynamics in the tail of the smeared transition. The long-time decay of the density (starting from a state with $\rho = 1$) is dominated by the rare regions while the bulk contribution decays exponentially. According to finite-size scaling [27], the behaviour of the correlation time ξ_t of a single rare region of size L_r in the vicinity of the clean bulk critical point can be modelled by

$$\xi_t(\Delta, L_r) \sim L_r^{(z\nu_\perp - \tilde{z}\tilde{\nu}_\perp)/\nu_\perp} \left|\Delta - A L_r^{-1/\nu_\perp}\right|^{-\tilde{z}\tilde{\nu}_\perp}. \tag{6}$$

Here $\Delta = \lambda - \lambda_c^0 > 0$, z is the d-dimensional bulk dynamical critical exponent, and $\tilde{\nu}_\perp$ and $\tilde{z}$ are the correlation length and dynamical exponents of a d_r-dimensional system. To exponential accuracy, the time dependence of the total density is given by

$$\rho(\lambda, t) \sim \int \mathrm{d}L_r \exp\left[-\tilde{p} L_r^{d_r} - Dt/\xi_t(\Delta, L_r)\right] \tag{7}$$

where D is a constant.

Let us first consider the time evolution at the clean critical point $\lambda = \lambda_c^0$. For $\Delta = 0$, the correlation time (6) simplifies to $\xi_t \sim L_r^z$. Using the saddle point method to evaluate the integral (7), we find the leading long-time decay of the density to be given by a stretched exponential,

$$\ln \rho(t) \sim -\tilde{p}^{z/(d_r+z)} t^{d_r/(d_r+z)}. \tag{8}$$

For $\lambda < \lambda_c^0$, i.e, in the absorbing phase, the correlation time of the largest islands does not diverge but is cut off by the distance from the clean critical point, $\xi_t \sim \Delta^{-z\nu}$. The large islands with this correlation time dominate the variational integral (7). This leads to a simple exponential decay with a decay constant $\tau \sim \Delta^{-z\nu}$.

The most interesting case is $\lambda > \lambda_c^0$, i.e., the tail region of the smeared transition. Here, we repeat the saddle point analysis with the full expression (6) for the correlation time. For intermediate times $t < t_x \sim \left(\lambda - \lambda_c^0\right)^{-(d_r+z)\nu_\perp}$ the decay of the average density is still given by the stretched exponential (8). For times larger than the crossover time t_x the system realizes that some of the rare regions are in the active phase and contribute to a finite-steady state density. The approach of the average density to this steady state value is characterized by a power law.

$$\rho(t) - \rho(\infty) \sim t^{-\psi}. \tag{9}$$

The value of ψ cannot be found by our methods since it depends on the neglected nonuniversal pre-exponential factors.

3. Monte Carlo simulations

3.1. Simulation method

We now illustrate the smearing of the phase transition by extensive computer simulation results for a 2d contact process with linear defects ($d_{\mathrm{cor}} = d_r = 1$). There are a number of different ways to actually implement the contact process on the computer (all equivalent with respect to the universal behaviour). We follow the widely used algorithm described, e.g., by Dickman [28]. Runs start at time $t = 0$ from some configuration of occupied and empty sites. Each event consists of randomly selecting an occupied site $\mathbf{r}$ from a list of all N_p occupied sites, selecting a process: creation with probability $\lambda(\mathbf{r}_r)/[1 + \lambda(\mathbf{r}_r)]$ or annihilation with probability $1/[1 + \lambda(\mathbf{r}_r)]$ and, for creation, selecting one of the neighbouring sites of $\mathbf{r}$. The creation succeeds, if this neighbour is empty. The time increment associated with this event is $1/N_p$.

Using this algorithm, we have performed simulations for linear system sizes up to $L = 3000$ and impurity concentrations $p = 0.2$, 0.25, 0.3, 0.35 and 0.4. The relative strength of the birth rate on the impurities was $c = 0.2$ for all simulations. The data presented below represent averages of 200 disorder realizations. Because of the large system sizes and the high number of realizations, the statistical errors are very low. The *relative* statistical error of the average density ranges from $\delta\rho/\rho \approx 10^{-4}$ at high densities to $\delta\rho/\rho \approx 10^{-2}$ for $\rho \approx 10^{-3}$ and to $\delta\rho/\rho \approx 10^{-1}$ for the lowest shown densities $\rho \approx 10^{-6}$. Except at these lowest densities, the error is smaller than or comparable with the line width in the figures.

We have chosen the above parameters, namely, a low concentration of impurities which have a birth rate much smaller than the bulk, because these conditions are favourable for observing the smeared transition in a finite-size simulation. If p was too large, the exponential drop-offs in equations (5) and (8) would be very steep and hard to observe over a significant range of λ or t, respectively. If c was too close to one, clean critical fluctuations would mask the tail of the smeared transition.

3.2. Time evolution

In this subsection, we discuss the time evolution of the density starting from a completely occupied lattice, $\rho(0) = 1$. Figure 1 presents an overview of the behaviour of a system with impurity concentration $p = 0.2$, system size $L = 3000$ and several birth rates from $\lambda = 1.62 \ldots 1.68$. The clean critical point is at $\lambda_c^0 = 1.6488$ [20]. The figure shows that the long-time decay of the density in the absorbing phase, $\lambda < \lambda_c^0$, is approximately exponential, in agreement with the expectation discussed after equation (8). The decay constant of this exponential increases with decreasing λ. In contrast, for $\lambda > \lambda_c^0$ the density approaches a nonzero value in the long-time limit. Close to λ_c^0, the density appears to decay, but slower than exponentially.

According to equation (8), the behaviour right at the clean critical point, $\lambda = \lambda_c^0$, is expected to be a stretched exponential rather than a simple exponential decay. To shed more light on the time evolution at λ_c^0, the behaviour of $\ln\rho$ as a function of $t^{d_r/(d_r+z)}$ is presented in the left panel of figure 2 for several impurity concentrations p. For our system, $d_r/(d_r + z) = 0.362$ with $z = 1.76$ being the dynamical exponent of the clean 2d contact process [29]. The figure shows that the data follow a stretched exponential behaviour $\ln\rho = -Et^{0.362}$ over

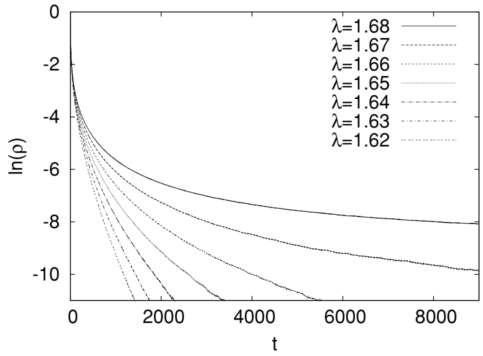

Figure 1. Overview of the time evolution of the density ρ for a system with $L = 3000$ and $p = 0.2$ and several birth rates ($\lambda = 1.68, \ldots, 1.62$ from top to bottom) in the vicinity of the clean critical point $\lambda_c^0 = 1.6488$.

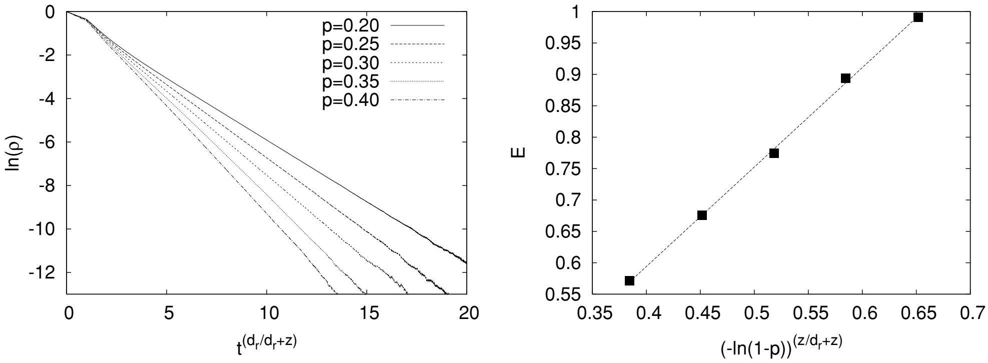

Figure 2. Left: logarithm of the density at the clean critical point λ_c^0 as a function of $t^{d_r/(d_r+z)} = t^{0.362}$ for several impurity concentrations ($p = 0.2, \ldots, 0.4$ from top to bottom) and $L = 3000$. The long-time behaviour follows a stretched exponential $\ln \rho = -Et^{0.362}$. Right: decay constant E of the stretched exponential as a function of $[-\ln(1-p)]^{z/(d_r+z)} = [-\ln(1-p)]^{0.638}$.

more than three orders of magnitude in ρ, in good agreement with equation (8) (the very slight deviation of the curves from a straight line can be attributed to the pre-exponential factors neglected in the extremal statistics theory). The right panel of figure 2 shows the decay constant E, i.e., the slope of these curves as a function of $\tilde{p} = -\ln(1-p)$. In good approximation, the values follow the power law $E \sim \tilde{p}^{z/(d_r+z)} = \tilde{p}^{0.638}$ predicted in (8).

In the tail of the smeared transition, i.e. for $\lambda > \lambda_c^0$ the density has a constant nonzero value $\rho_{\mathrm{st}} = \rho(\infty)$ in the long-time limit. Figure 3 illustrates the approach of the density to this value. It shows $\ln[\rho(t) - \rho_{\mathrm{st}}]$ as a function of $\ln(t)$ for several λ. The long-time behaviour is clearly of power-law type, but the exponent depends on λ, i.e., it is nonuniversal. These results agree with the corresponding prediction in equation (9).

3.3. Stationary state

In this subsection we present and analyse the simulation results for the stationary state in the tail of the smeared transition, $\lambda > \lambda_c^0$. Figure 4 shows a comparison of the stationary

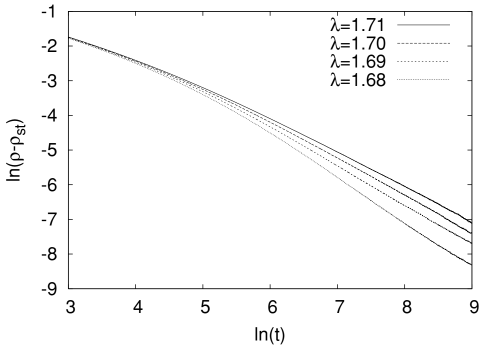

Figure 3. Double-logarithmic plot of the approach of the density to its nonzero stationary value in the tail of the smeared transition for a system with $p = 0.2$ and $L = 3000$ and birth rate $\lambda = 1.71, 1.70, 1.69, 1.68$ (top to bottom). The long-time behaviour is of power-law type, $(\rho(t) - \rho_{\rm st}) \sim t^{-\psi}$. Fits yield exponents of approximately 1.00, 1.08, 1.12 and 1.28, respectively.

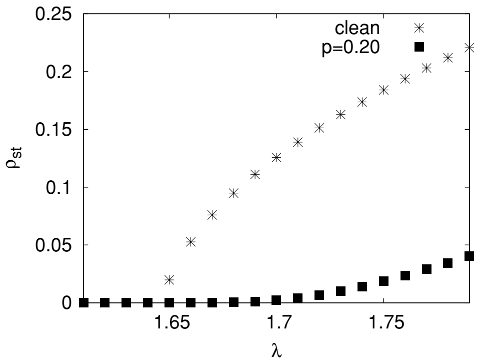

Figure 4. Stationary density $\rho_{\rm st}$ as a function of birth rate λ for a clean system and a system with impurity concentration $p = 0.2$. System size is $L = 1000$.

density $\rho_{\rm st}$ as a function of λ between the clean system and a dirty system with $p = 0.2$. The clean system ($p = 0$) has a sharp phase transition with a power-law singularity of the density, $\rho_{\rm st} \sim \left(\lambda - \lambda_c^0\right)^{\beta}$ with $\beta \approx 0.58$ in agreement with the literature [20]. In contrast, in the dirty system, the density increases much more slowly with λ after crossing the clean critical point. This suggests either a critical point with a very large exponent β or exponential behaviour.

Let us now investigate the behaviour of the dirty system in the low-density tail more closely. In figure 5, we plot $\ln \rho_{\rm st}$ as a function of $\left(\lambda - \lambda_c^0\right)^{-d_r \nu_\perp}$ for several impurity concentrations p, as suggested by equation (5). The data in the left panel of figure 5 show that the density tail is indeed exponential, following the prediction $\ln \rho_{\rm st} = -B\left(\lambda - \lambda_c^0\right)^{-d_r \nu_\perp}$ over at least two orders of magnitude in $\rho_{\rm st}$. (The clean 2d spatial correlation length exponent is $\nu_\perp = 0.734$ [29].) Fits of the data to equation (5) are used to determine the decay constants B. The right panel of figure 5 shows these decays constants as function of $\tilde{p} = -\ln(1 - p)$. The dependence is close to linear, as predicted below equation (4) (slight deviations from the theoretical prediction can again be attributed to the pre-exponential terms neglected in the extremal statistics theory).

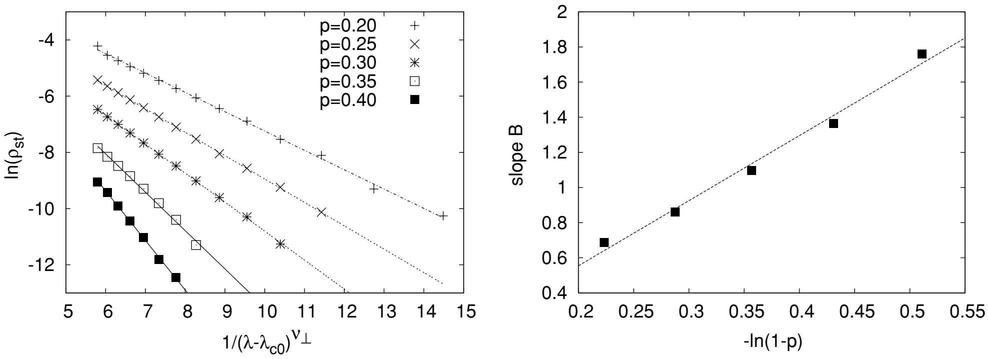

Figure 5. Left: logarithm of the stationary density ρ_{st} as a function of $(\lambda - \lambda_c^0)^{-d_r \nu_\perp} = (\lambda - \lambda_c^0)^{-0.734}$ for several impurity concentrations p and $L = 3000$. The straight lines are fits to equation (5). Right: decay constant B as a function of $-\ln(1 - p)$.

4. Discussion and conclusions

To summarize, we have provided extensive numerical evidence that extended impurities destroy the sharp nonequilibrium phase transition in the contact process by smearing and lead to a (nonuniversal) exponential dependence of the density and other quantities on the control parameter. These results are in agreement with the predictions of [26] which were based on extremal statistics arguments and mean-field theory. In this section, we first relate our findings to a power-counting analysis of the corresponding field theory. We then compare our smeared phase transition to the more conventional Griffiths effects in the contact process with point-like defects [1, 17], and discuss general implications for theory and experiment.

The field-theoretic formulation of the contact process [30, 31] is the so-called Reggeon field theory which was originally studied in the context of hadronic interactions at ultra-relativistic energies (for a review see, e.g., [32]). In appropriate units, its action reads

$$S = \int \mathrm{d}^d r \, \mathrm{d}t \tilde{\phi} \left[\partial_t - \kappa - \nabla^2 + \frac{\Gamma}{2}(\phi - \tilde{\phi}) \right] \phi \tag{10}$$

where $\phi(\mathbf{r}, t)$ represents the density while $\tilde{\phi}(\mathbf{r}, t)$ is the Martin–Siggia–Rosen response field and κ denotes the bare distance from the transition. A simple power counting analysis for the scale dimension of Γ at the Gaussian fixed point yields $[\Gamma] = 4 - d$, i.e., the upper critical dimension of this field theory is $d_c^+ = 4$. Spatially quenched disorder (both uncorrelated or correlated) can be taken into account by adding a term

$$S_{\mathrm{dis}} = \gamma \int \mathrm{d}^{d_r} r_r \left[\int \mathrm{d}^{d_{\mathrm{cor}}} r_{\mathrm{cor}} \, \mathrm{d}t \tilde{\phi} \phi \right]^2 \tag{11}$$

where the outer integral is over the uncorrelated directions $\mathbf{r}_r$ while the inner spatial integrals are over the correlated directions $\mathbf{r}_{\mathrm{cor}}$ (see [18] for the uncorrelated case $d_{\mathrm{cor}} = 0$). Power counting for the scale dimension of γ gives $[\gamma] = 4 - d + d_{\mathrm{cor}}$. Uncorrelated disorder is marginal at $d = d_c^+ = 4$, but disorder correlations increase the scale dimension of γ making the disorder term renormalization-group relevant. The power-counting analysis thus predicts stronger effects for correlated disorder than for point-like disorder, in agreement with our results. Let us emphasize, however, that the smeared phase transition scenario found in this paper cannot be obtained in a perturbative analysis of the Reggeon field theory because the rare regions are non-perturbative degrees of freedom.

Both conventional Griffiths effects and the smearing scenario found in this paper are caused by rare large spatial regions which are locally in the active phase even if the bulk system is not. The difference between Griffiths effects and the smearing of the transition is the result of disorder correlations. For point-like defects, i.e., uncorrelated disorder, the rare regions are of finite size and cannot undergo a true phase transition. Instead, they fluctuate slowly which gives rise to Griffiths effects. In contrast, if the rare regions are infinite in at least one dimension, a stronger effect occurs: each rare region can independently undergo the phase transition and develop a nonzero steady state density. This leads to a smearing of the global transition.

The smearing mechanism found here relies only on the existence of a true phase transition on an isolated rare region. It should therefore apply not only to the directed percolation universality class, but to an entire family of nonequilibrium universality classes for spreading processes and reaction–diffusion systems. Note that while the presence or absence of smearing is universal in the sense of critical phenomena (it depends on symmetries and dimensionality only), the functional form of the density and other observables is *not* universal, it depends on the details of the disorder distribution [4].

Smearing phenomena similar to that found here can also occur at equilibrium phase transitions. At quantum phase transitions in itinerant electron systems, even point-like impurities can lead to smearing [5] (the necessary disorder correlations are in imaginary time direction). In contrast, for the classical Ising (Heisenberg) universality class, the impurities have to be at least 2d (3d) for the transition to be smeared which makes the phenomenon less likely to be observed [4].

In the context of our findings it is worth noting that, despite its ubiquity in theory and simulations, clearcut experimental realizations of the directed percolation universality class are strangely lacking [33]. To the best of our knowledge, the only verification so far has been found in the spatio-temporal intermittency in ferrofluidic spikes [34]. We suggest that the disorder-induced smearing found in this paper may explain the striking absence of directed percolation scaling [33] in at least some of the experiments.

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