Theory of Branching and Annihilating Random Walks

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A systematic theory for the diffusion-limited reaction processes $A + A \to 0$ and $A \to (m + 1)A$ is developed. Fluctuations are taken into account via the field-theoretic dynamical renormalization group. For even m, the mean field rate equation, which predicts only an active phase, remains qualitatively correct near $d_c = 2$ dimensions; but below $d_c' \approx 4/3$ a nontrivial transition to an inactive phase governed by power law behavior appears. For odd m, there is a dynamic phase transition for any $d \leq 2$ which is described by the directed percolation universality class. [S0031-9007(96)01800-5]

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Nonequilibrium models with an extensive number of degrees of freedom whose dynamics violates detailed balance occur in studies of many biological, chemical, and physical systems. Like equilibrium systems, their stationary states may exhibit phase transitions which in many cases appear to fall into distinct classes characterized by universal quantities such as critical exponents. One of the most common such classes is that exemplified by *directed percolation* (DP) [1]. This represents a transition from a nontrivial "active" steady state to an absorbing "inactive" state with no fluctuations. Many nonequilibrium phase transitions appear to belong to this universality class, e.g., the contact process [2], the dimer poisoning problem in the Ziff-Gulari-Barshad model [3], and autocatalytic reaction models [4]. The universal properties of the DP transition are theoretically well understood in the context of a renormalization group (RG) analysis based on an expansion around mean field theory below the upper critical dimension $d_c = 4$ [5].

More recently a class of models has been studied which, in certain cases, appear as exceptions to the general rule that such transitions should fall into the DP universality class. These include a probabilistic cellular automaton model [6], certain kinetic Ising models [7,8], and an interacting monomer-dimer model [9]. In one dimension the dynamics of these is equivalent to a class of models called *branching and annihilating random walks* (BARWs) [10–12], which also have a natural generalization to higher dimensions. In the language of reaction-diffusion systems, BARWs describe the stochastic dynamics of a single species of particles A undergoing three basic processes: diffusion, often modeled by a random walk on a lattice and characterized by a diffusion coefficient D; an annihilation reaction $A + A \to 0$ when particles are close (or on the same site), at rate λ; and a branching process $A \to (m + 1)A$ (where m is a positive integer), at rate σ_m. The above-mentioned one-dimensional models all correspond to the case $m = 2$. For the kinetic Ising model, the particles A are to be identified with the domain walls, and the transition to the inactive state corresponds to the ordering of the Ising spins [7,8]. In general, this new universality class has been observed in $d = 1$ for *even* values of m, when the number of particles is locally conserved modulo 2. When m is *odd*, the DP values of the exponents appear to be realized. (It should be remarked that several of the models which have been studied do not contain three independent parameters corresponding to D, λ, and σ_m so that it may occur that the actual transition is inaccessible. This appears to be so for the simplest lattice BARW model with $m = 2$, which is always in the inactive phase [10].)

Besides the appearance of a new universality class, another issue which clearly requires theoretical explanation is the *occurrence* of a transition at a finite value of σ_m. For the mean field rate equation for the average density

$$\dot{n}(t) = -2\lambda n(t)^2 + m\sigma_m n(t) \tag{1}$$

predicts a nonzero steady state density $m\sigma_m/2\lambda$, so that this state should be *active* for all $\sigma_m > 0$, in contrast to what is in fact observed for $d = 1$. It is, however, known that fluctuation effects render the mean field description of the pure annihilation problem ($\sigma_m = 0$) qualitatively incorrect for $d \leq 2$ [13]. Therefore, a detailed theory has to demonstrate how these are also responsible for moving the critical value of σ_m away from zero.

In this Letter, we describe the first systematic theory of these phenomena (details will be presented elsewhere [14]). It is based on the field-theoretic RG analysis which has proven successful for the DP problem [5]; however, we correct an important error which was made in an earlier investigation along the same lines [6]. A summary of our main results follows.

(a) Even m.—For $d > 2$ the mean field description (1) is qualitatively correct in that the transition occurs at $\sigma_m = 0$. The density in the active phase vanishes as $n \propto \sigma_m$, with calculable logarithmic corrections in two dimensions. As d is lowered below 2, the transition first continues to occur at $\sigma_m = 0$, with modified critical exponents, until a *second critical dimension* $d_c' \approx 4/3$ is reached. Below this, and in particular for $d = 1$, there appears a nontrivial transition at $\sigma_c > 0$ from the active phase to an inactive phase in which the density decays asymptotically as $n \propto t^{-d/2}$. Because of the existence of *two* critical dimensionalities, this new universality class apparently has no simple mean field limit, close

to which the fluctuations can be controlled. We are therefore unable to generate a systematic ϵ expansion for the critical exponents. The truncated loop expansion in fixed dimension seems to provide at least a qualitative description of the transition; however, as there exists no small expansion parameter, the actual values for the critical exponents to one-loop order are rather inaccurate. The RG analysis also shows that higher values of m inevitably generate an effective $m = 2$ reaction under renormalization, and this is always the most relevant term. Therefore all such processes with even m fall into the same universality class. We have also considered an N species generalization of the $m = 2$ model. The RG analysis shows that for $N > 1$ the critical behavior is that of the $N \to \infty$ limit, which is exactly solvable but always in the *active* phase for $\sigma_2 > 0$, with critical exponents being described by yet another universality class.

(b) Odd m.—The case $m = 1$ here is typical. Under renormalization, a spontaneous decay process $A \to 0$ is generated for arbitrarily small branching rates, by the combined reactions $A \to 2A$, $2A \to 0$, so that the density decays *exponentially,* as in the inactive phase of DP. We find this to occur for $d < 2$, when the pure annihilation process is relevant. For $d \geq 2$, however, the situation is more subtle. The RG analysis in this case predicts that there is in fact a nontrivial transition even at $d_c = 2$, with $\sigma_c \sim De^{-4\pi D/\lambda}$, while it is absent for $d > 2$. Analysis of the effective theory for $d \leq 2$ then shows that the subsequent transition at larger values of σ_1 is in the DP universality class, as is observed in simulations [10,11].

The field-theoretic analysis of these problems begins from the "second-quantized" approach to classical stochastic particle systems which is well known and has been described in detail elsewhere [13,15]. Annihilation and creation operators a_i and $a_i^\dagger$, satisfying the usual boson commutation relations, are introduced at each site i of the lattice, and the time-dependent state vector $|\Psi(t)\rangle \equiv \sum_{\{n_i\}} p(\{n_i\};t) \prod_i a_i^{\dagger n_i}|0\rangle$ is constructed from the probabilities $p(\{n_i\};t)$. The (classical) master equation satisfied by these may then be recast as a Schrödinger-like equation with a time evolution operator which, in this example, has the form $H = H_d + H_a + H_b + H_T$, where

$$H_d = D\sum_{(ij)}(a_i^\dagger - a_j^\dagger)(a_i - a_j)\,, \tag{2}$$

$$H_a = -\lambda\sum_i(a_i^2 - a_i^{\dagger 2}a_i^2)\,, \tag{3}$$

$$H_b = -\sigma_m\sum_i(a_i^{\dagger m+1}a_i - a_i^\dagger a_i)\,, \tag{4}$$

$$H_T = -\tau\sum_i(a_i^{\dagger 2} - 1)\,. \tag{5}$$

The last term corresponds to a constant creation of pairs of particles, simulating the effects of finite temperature in the kinetic Ising model [8]. Finally, utilizing the coherent-state path integral formalism, the "quantum many particle" Hamiltonian H can be cast into a field theory which describes BARW processes *including* fluctuation effects. Note that no additional assumptions, specifically regarding the form of the noise correlations in an extension of Eq. (1) to an effective Langevin equation, had to be invoked in this derivation.

When m is *even,* there is a formal symmetry of H under changing the signs of all the a_i and $a_i^\dagger$ simultaneously: this corresponds to the conservation of particle number modulo 2. However, in this formalism, expectation values of operators such as the local density $n_j = a_j^\dagger a_j$, for example, are given by matrix elements of the form $\langle 0|e^{\sum_i a_i}n_j e^{-Ht}|\Psi(0)\rangle$, and in order to use the time-dependent perturbation theory and Wick's theorem it is conventional to commute the factor $e^{\sum_i a_i}$ through. This is equivalent to applying the formal shift $a_i^\dagger \to 1 + a_i^\dagger$ in H. Yet this obscures the above symmetry, and if, in accordance with the usual naive power counting arguments near the upper critical dimension, higher order quartic terms in H are then ignored, it becomes completely lost. This led the authors of Ref. [6] to the erroneous conclusion that, near $d = 4$, the transition should be in the DP universality class *irrespective* of the parity of m.

However, it is imperative in any RG analysis to preserve all known symmetries of the system. In the present case, this may be done by observing that the RG equations themselves (as opposed to the calculations of observables such as the density) should be independent of which basis is used, and it is therefore possible, and, indeed, necessary, to perform the computations in the representation of the model in which the symmetry is manifest. The methods for doing this are standard, and will be described in detail elsewhere [14]. The case $\sigma_m = \tau = 0$, corresponding to a pure annihilation process, has already been analyzed in [13]. The RG equation for the flow of the dimensionless coupling $\ell \equiv C_d\lambda/D\kappa^\epsilon$, where κ is a normalization wave number, $C_d = \Gamma(2 - d/2)/2^{d-1}\pi^{d/2}$ a geometric factor, and $\epsilon = 2 - d$, under a rescaling factor e^l, is given by $d\ell/dl = \epsilon\ell - \ell^2$, which is exact at one loop. For $d < 2$ the late time behavior is controlled by the nontrivial fixed point at $\ell^* = \epsilon$, leading to an asymptotic particle density decay according to $n(t) \propto t^{-d/2}$.

The first question to be addressed is whether the branching rate σ_m is relevant at the pure annihilation fixed point, i.e., whether its RG eigenvalue y_σ is positive. If so, the late time behavior must differ from that of the pure annihilation process, indicating that the active phase is reached immediately. For $d \geq 2$ we find $y_\sigma = 2$ from simple power counting, so indeed σ_m is relevant. The density in the active phase vanishes according to the mean field result $n \propto \sigma_m$. For $d < 2$, to one-loop order, $y_\sigma = 2 - [m(m+1)/2]\ell + O(\ell^2)$, so that σ_m remains relevant at the annihilation fixed point $\ell^* = \epsilon$ just below $d = 2$, with the lower values of m being the most relevant. Since these lower allowed values of m

inevitably become generated whenever the annihilation rate is nonzero, we conclude that the cases with m even will always fall into the universality class of $m = 2$, while m odd will generate $m = 1$ and $m = -1$. The latter is always relevant, and, as we shall see below, is responsible for the crossover to the DP universality class. For the time being we therefore restrict our attention to the case of even m. For $d = 2$ the marginality of ℓ is responsible for logarithmic corrections to mean field theory, which for $m = 2$ take the form $n \propto \sigma/[\ln(1/\sigma)]^2$.

The above result for y_σ is valid only close to $d = 2$. Fortunately it is possible to compute it *exactly* in one dimension, at the pure annihilation fixed point. The latter corresponds to the limit of infinite bare coupling λ [13]. The multiparticle states then effectively propagate as hard-core bosons in between the annihilation and branching processes, and so, in one dimension, behave like free fermions. On the lattice, this limit makes sense only if we define the branching process as placing the m offspring on different but neighboring sites. The branching contribution to H, in terms of these fermionic operators c_i and $c_i^\dagger$, thus acquires the form $H_b = \sigma_m \sum_i \prod_{j=-m/2}^{m/2} c_{i+j}^\dagger c_i$. The continuum limit of this expression, found by performing a Taylor expansion in powers of the lattice spacing a_0, will be different from the bosonic case because the anticommuting nature of the $c_i^\dagger$ allows each derivative to appear only *once*. The lowest order term has the form $a_0^{m(m+1)/2} c^\dagger(\partial c^\dagger)(\partial^2 c^\dagger)\cdots(\partial^m c^\dagger)c$, with the result that the effective expansion parameter $\tilde{\sigma}_m \equiv a_0^{m(m+1)/2}\sigma_m$ has a modified scaling dimension. This leads to the result (which may be confirmed by other less formal methods) that $y_\sigma = 2 - m(m+1)/2$ *exactly* in $d = 1$. Thus, for reasons we do not understand, the $O(\epsilon)$ result appears to be exact in $d = 1$, and y_σ changes sign at a value of $d = d_c' \approx 4/3$ for $m = 2$, if the higher order terms continue to be small. In $d = 1$, $y_\sigma < 0$ for all the even values of m. This establishes the result that the late time behavior for small values of σ_m is controlled by the annihilation fixed point, so that $n(t) \propto t^{-1/2}$. In the inactive phase, the system is composed of a set of highly *anticorrelated* bunches of odd numbers of particles, the spatial distribution of which, upon coarse graining, looks like that of single particles in the pure annihilation process.

Clearly, the above scenario cannot be obtained in any finite order of an expansion near $d_c = 2$. We have therefore performed a truncated loop expansion at fixed dimension, retaining the full dependence on σ, which appears both as a vertex and as a mass term. To one loop order, the RG flow equations for the renormalized reaction rates $\ell = C_d \lambda / D\kappa^{2-d}$ and $s = \sigma/D\kappa^2$ read ($m = 2$)

$$d\ell/dl = \ell[2 - d - \ell/(1+s)^{2-d/2}], \tag{6}$$

$$ds/dl = s[2 - 3\ell/(1+s)^{2-d/2}]. \tag{7}$$

For $s \to 0$, the annihilation fixed point $\ell^* = 2 - d$ of the inactive phase is recovered, while for $s \to \infty$ the loop contributions to the anomalous dimensions vanish, and the flow approaches a Gaussian fixed point describing the active phase. For large s, the effective coupling in Eqs. (6) and (7) becomes $g \equiv \ell/s^{2-d/2}$ (see Sec. III of Ref. [16]), whose flow is given by $dg/dl = 2g - [(10-3d)/2]g^2 \equiv -\beta(g)$. In addition to the stable Gaussian fixed point at $g = 0$ there is a nontrivial *unstable* one at $g^* = 4/(10-3d)$ describing the phase transition. At this order there is neither field nor diffusion constant renormalization, giving a dynamic exponent $z \approx 2$. However, because the mean field density $n \sim \sigma/\lambda$ and the spatial correlation length $\xi_\perp \sim \sigma^{-1/2}$ depend not just on g but also on the dangerous irrelevant variable s^{-1}, the critical exponents describing the approach to the critical point in the active phase depend not only on $y_\varepsilon \equiv \beta'(g^*)$, describing the distance from the critical point $\varepsilon \equiv (g^* - g)/g^*$, but also on $y_\lambda \approx 2 - d - g^*$ and $y_\sigma \approx 2 - 3g^*$. As a result we find that $n \sim \varepsilon^\beta$, with $\beta = (d + y_\lambda - y_\sigma)/y_\varepsilon \approx 4/(10-3d)$, and $\xi_\perp \sim \varepsilon^{-\nu_\perp}$, with $\nu_\perp = (1 - y_\sigma)/y_\varepsilon \approx 3/(10-3d)$. The truncated one-loop approximation thus seems to provide a qualitatively correct picture of the transition, although the actual numerical values of these exponents in one dimension are rather poor as compared to simulation results [8]; this is not very surprising, however, as there is no small expansion parameter present here. In addition, we cannot really access those exponents that describe the behavior *at* the critical point, as the density might depend nonanalytically on σ there; this also precludes a sound derivation of scaling relations [8] connecting these with the above exponents describing the active phase.

A better result is obtained for the exponent $\nu_\tau \equiv 1/y_\tau$ describing the divergence of the correlation length as the pair creation rate $\tau \to 0$ at the critical point $\varepsilon = 0$. The one-loop flow equation for τ reads

$$d\tau/dl = \tau[d + 2 - \ell/(1+s)^{2-d/2}], \tag{8}$$

and hence in the inactive phase, or at the critical point $\sigma = 0$ for $d > d_c'$, one has $\nu_\tau = 1/2d$, while at the nontrivial phase transition for $d < d_c'$ the result is $\nu_\tau \approx (10-3d)/(16+4d-3d^2)$. In one dimension, $\nu_\tau \approx 7/17$, which is in fair agreement with simulations [8].

We have also investigated an N species generalization of the $m = 2$ problem, defined by the processes $2A^\alpha \to 0$, at rate λ/N, $A^\alpha \to 3A^\alpha$, at rate σ, and $A^\alpha \to A^\alpha + 2A^\beta$, $\beta \neq \alpha$, at rate $\sigma'/(N-1)$. To one-loop order at the annihilation fixed point the RG eigenvalue of the additional branching process becomes $y_{\sigma'} = 2 - \ell$, which is therefore *more relevant* than the original reaction with rate σ. We have chosen the above N component version, because for $N \to \infty$, the ensuing theory (with $\sigma = 0$) can be solved exactly; physically this limit corresponds to the situation where each particle may annihilate only with its sibling. The resulting critical point remains at $\sigma_c = 0$ for all d, and its universality class, *distinct* from the previously discussed ones, is characterized by the mean field exponents $z = 2$, $\beta = 1$, and as a consequence of the now *exact* result $y_{\sigma'} = 2 - \ell$, we find $\nu_\perp \equiv 1/y_{\sigma'} = 1/d$, using $\ell^* = 2 - d$ for $d \leq 2$.

We now return to the case of odd m. As argued above, fluctuations generate a spontaneous single-particle decay process, and the *effective* interactions at a given site acquire the form

$$\mu(a^\dagger - 1)a - \sigma(a^\dagger - 1)a^\dagger a + \lambda(a^{\dagger 2} - 1)a^2. \quad (9)$$

When the single-particle decay rate $\mu \neq 0$, it is convenient to remove the linear term in a by the shift $a^\dagger \to 1 + a^\dagger$ mentioned earlier. This results in the interaction Hamiltonian

$$\tilde{H}_{\rm eff}^{\rm int} = (\mu - \sigma)a^\dagger a - \sigma a^{\dagger 2} a + 2\lambda a^\dagger a^2 + \lambda a^{\dagger 2} a^2. \quad (10)$$

If we now neglect the quartic term (justifiable in this case since there is no "parity" symmetry that must be preserved), we find precisely the interaction Hamiltonian used to characterize DP [5]. The transition occurs when the renormalized version of the mass term $\mu_R - \sigma_R$ vanishes. The question of whether this actually happens for allowed values of the bare parameters σ and λ depends on the way these are renormalized, and this may be studied close to $d = 2$. It is simpler to work in the unshifted version (9), where it is straightforward to identify the most singular ("bubble") diagrams in powers of ϵ^{-1} at a given order in λ. The mass in the shifted DP Hamiltonian (10) then becomes $\mu_R - \sigma_R = \sigma(I_d - 1)/(I_d + 1)$, where $I_d \equiv (C_d\lambda/D\epsilon)[(\mu_R + \sigma_R)/D]^{-\epsilon/2} = (C_d\lambda/D\epsilon)(\sigma/D)^{-\epsilon/2}$ because $\mu_R + \sigma_R = \sigma$ in this approximation. For sufficiently small σ, this is positive, indicating that the system is in the inactive phase with an *exponential* decay of the density. The transition to the active phase occurs at $\sigma_c = D(C_d\lambda/D\epsilon)^{2/\epsilon}$. Although this result is accurate only to leading order in ϵ, the general feature of a transition at a finite value of σ in the DP universality class should persist to $d = 1$. For $d = 2$ the transition is seen to continue to occur at a finite value $\sigma_c \sim De^{-4\pi D/\lambda}$, as $\lambda \to 0$. However, for larger d, the annihilation rate λ which drives the generation of the process $A \to 0$, essential for the DP inactive state, becomes irrelevant, and one may use the same set of diagrams to argue that there is now no transition, at least for small λ.

The same result can be obtained in the framework of an RG calculation similar to that invoked for m even. This method yields for $m = 3$ the same qualitative picture as for $m = 1$, but the transition moves closer to the mean field critical point, with $\sigma_c \sim De^{-5.68\pi D/\lambda}$ [14], and we expect this tendency to hold for larger odd values of m, in accord with numerical simulations [10,11].

To summarize, we have provided the first analytic theory of branching and annihilating random walks which explains most of their observed behavior. We have shown that the fluctuations responsible for the failure of mean field theory in the pure annihilation process for $d \leq 2$ are also responsible for shifting the critical value of the branching rate away from zero. For m odd this occurs for all $d \leq 2$, with the subsequent transition being in the DP universality class, while for m even this effect is postponed to lower dimensions $d < d_c' \approx 4/3$. Our theory correctly takes account of the symmetry in this case, but is so far unable to yield accurate estimates of the critical exponents in $d = 1$. However, a truncated loop expansion appears to provide at least a qualitative picture of the transition. It would of course be desirable to find some other controlled approximation scheme in which to approach this problem. Our investigation of an N species generalization of the $m = 2$ reaction failed to provide us with additional insight in the single species case, but instead uncovered yet another new universality class for $N > 1$, with $\sigma_c = 0$ and governed by the exponents of the exactly solvable $N \to \infty$ limit. This underlines the importance of fluctuations and correlation effects in reaction-diffusion systems at low dimensions, which may lead to remarkably rich nonequilibrium phase diagrams.

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