Nonperturbative Renormalization-Group Study of Reaction-Diffusion Processes

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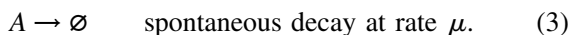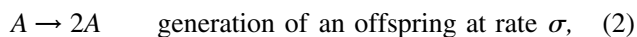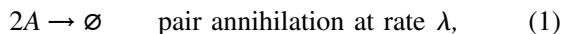(Received 22 September 2003; published 13 May 2004)

We generalize nonperturbative renormalization group methods to nonequilibrium critical phenomena. Within this formalism, reaction-diffusion processes are described by a scale-dependent effective action, the flow of which is derived. We investigate branching and annihilating random walks with an odd number of offspring. Along with recovering their universal physics (described by the directed percolation universality class), we determine their phase diagrams and predict that a transition occurs even in three dimensions, contrarily to what perturbation theory suggests.

The description of many physical, chemical, and biological systems resorts to nonequilibrium many-particle models. Their dynamical evolution is governed by a Markov process ruled by microscopic transition probabilities which violate detailed balance. The ensuing macroscopic behaviors are hence intrinsically much richer than in equilibrium. Many models exhibit phase transitions between stationary states, which have unveiled the existence of universal properties. The characterization of the nonequilibrium universality classes constitutes a prevalent issue of statistical mechanics. In this respect, reaction-diffusion processes provide a simple and thus valuable framework to investigate nonequilibrium critical phenomena. They generically describe diffusing particles that can undergo different microscopic reactions [1,2]. The most common universality class encountered is that of directed percolation (DP) [3,4]. It can be simply achieved through a reaction-diffusion model endowed with the following processes:

$$2A \to \varnothing \qquad \text{pair annihilation at rate } \lambda, \qquad (1)$$

$$A \to 2A \qquad \text{generation of an offspring at rate } \sigma, \qquad (2)$$

$$A \to \varnothing \qquad \text{spontaneous decay at rate } \mu. \qquad (3)$$

The competition between birth and death gives rise to a steady state where the density saturates at a constant value ρ. The system exhibits a continuous phase transition between an active (fluctuating) state where $\rho > 0$, and an inactive (absorbing) state where the density vanishes. In fact, a large variety of models, such as the contact process [5], Reggeon field theory in particle physics [6], the dimer poisoning [7], and the autocatalytic reaction models [8], show the same critical behavior.

Despite considerable successes, the general understanding of nonequilibrium phenomena suffers from the lack of a systematic theoretical framework. Indeed, out of equilibrium, the absence of a free-energy functional from

which to draw the probability distribution of steady states prevents the use of well-established equilibrium methods. Instead, the master equation should be solved, which is not feasible in general. Fortunately, it can often be cast into a path integral representation [9], rooting a field theory that can be probed with a dynamical renormalization group (RG). The usual perturbative techniques consist of expansions in series of a parameter. They have allowed us to achieve numerous advances in our theoretical understanding. Nevertheless, as they rely on the smallness of a parameter, their validity remains confined to the vicinity of critical dimensions or to weak coupling regimes.

We propose in this Letter a powerful alternative, based on a nonperturbative RG procedure (NPRG) [10–12]. This method avoids the previous pitfalls as it does not intrinsically depend on the magnitude of a parameter. Moreover, the microscopic interactions can be traced all along the NPRG flow, and related to the long-range properties, thus giving access to nonuniversal quantities, such as equations of state and critical temperatures [13]. In this work, we generalize the NPRG methods to nonequilibrium systems and derive very generic, model-independent RG flow equations for reaction-diffusion processes. We exploit these equations to investigate branching and annihilating random walks (BARW) with an odd number of offspring. We first recover their universal physics which belong to the DP universality class. Then, linking the density ρ of stationary states with the microscopic rates enables us to push further a recent analysis by Cardy and Täuber [14]. We predict, in particular, that a phase transition can occur in three dimensions, contrarily to what was conjectured.

The NPRG formalism—the effective average action method [10]—is a continuous implementation, on successive momentum shells, of Wilson's block-spin concept. For equilibrium systems, it consists in building a

sequence of effective actions Γ_k, at the running momentum scale k, interpolating between the microscopic Hamiltonian H of the system, and its Gibbs free energy Γ. This is achieved by adding to the partition function Z a masslike term ΔH_k that suppresses the propagation of the low-energy modes (with wave number $q < k$) while not affecting the high-energy ones ($q > k$). The corresponding free-energy $\log Z_k$, or its Legendre transform Γ_k, thus encompasses only the large momentum fluctuations. At the scale $k = \Lambda$, Λ^{-1} corresponding to the underlying lattice spacing, no fluctuation has yet been taken into account and $\Gamma_{k=\Lambda} = H$, while at $k = 0$, all fluctuations have been integrated out and $\Gamma_{k=0} = \Gamma$. An exact RG equation for the flow of Γ_k is easily derived and underlies the NPRG formalism [10]. We now generalize this formalism to out of equilibrium systems, for which partition function and Gibbs free energy no longer exist. Despite this lack, a path integral formulation of the dynamics can be set up, commonly involving an auxiliary response field $\bar{\phi}$, along with the usual field ϕ. It allows us to define a generating functional Z for the correlation functions, and one, Γ, for the one-particle irreducible correlation functions. These functionals constitute the building blocks of an out of equilibrium NPRG. We introduce in Z a scale-dependent term, analogous to ΔH_k:

$$Z_k[\bar{J}, J] = \int D\phi D\bar{\phi} e^{-S[\bar{\phi}, \phi] - \Delta S_k[\bar{\phi}, \phi] + \int J\phi + \int \bar{J}\bar{\phi}}, \quad (4)$$

where

$$\Delta S_k = \int \frac{d^d p}{(2\pi)^d} \frac{d\omega}{2\pi} \Phi(-p, -\omega) \hat{R}_k(p) \Phi^T(p, \omega), \quad (5)$$

Φ denoting the two-component vector $(\bar{\phi}, \phi)$. The 2×2 matrix $\hat{R}_k$ is symmetric with zeros on its diagonal and a masslike function $R_k(p)$ off its diagonal. The selection of modes is ensured by imposing that, on the one hand, $R_k(p) \sim k^2$ for $p \ll k$; that is R_k acts as an effective mass—an IR cutoff—for slow modes. On the other hand, one imposes that $R_k(p) \to 0$ for $p \gg k$, so that the rapid modes remain unaltered. In this work, we use $R_k(p) = (k^2 - p^2)\theta(k^2 - p^2)$ [15] which gives simple analytical expressions for the momentum integrals. We emphasize that no cutoff is necessary for time, since the corresponding integrals are regular and the frequency dependence can be integrated over (see below). The effective action Γ_k is defined through the appropriate Legendre transform $\Gamma_k + \log Z_k = \int J\psi + \bar{J}\bar{\psi} - \Delta S_k(\bar{\psi}, \psi)$, where ψ ($\bar{\psi}$) is the mean value of ϕ ($\bar{\phi}$), defined as the derivative of Z_k with respect to (wrt) J ($\bar{J}$). The mass term ΔS_k ensures that the proper limits $\Gamma_{k=\Lambda} = S$ and $\Gamma_{k=0} = \Gamma$ are recovered. The exact flow equation of Γ_k is then easily derived, similarly to the equilibrium calculation [10]:

$$\partial_k \Gamma_k(\bar{\psi}, \psi) = \tfrac{1}{2} \mathrm{Tr}\{[\hat{\Gamma}_k^{(2)} + \hat{R}_k]^{-1} \partial_k \hat{R}_k\}, \quad (6)$$

where $\hat{\Gamma}_k^{(2)}$ is the field dependent matrix of the second functional derivatives of Γ, and Tr stands for matrix trace over internal indices and integration over the internal momentum and frequency. Equation (6) is a functional equation which obviously cannot be solved exactly. To handle it, one has to *truncate* Γ_k. Since the critical physics corresponds to the long distance ($q \to 0$), long time ($\omega \to 0$) limit, a sensible truncation consists in expanding Γ_k in powers of gradients [10] and time derivatives. Retaining only the leading order in derivatives, the functional Γ_k for reaction-diffusion systems reads

$$\Gamma_k(\bar{\psi}, \psi) = \int d^d r dt [Z_k \bar{\psi}(\partial_t - D_k \nabla^2)\psi + V_k(\bar{\psi}, \psi)]. \quad (7)$$

In principle, the three functions V_k, Z_k, and D_k depend on the fields, and their functional form is dictated by the symmetries of the underlying dynamics. We study in the following the leading order approximation that consists of neglecting the field dependence of Z_k and D_k [10]. Thus, we consider only their k dependence, which accounts for the critical anomalous scalings of the fields, and of time. Indeed, the anomalous dimension η of the fields is defined such that at criticality, ψ and $\bar{\psi}$ scale as $k^{(d+\eta)/2}$. This definition induces that $\eta = -\partial \ln Z_k / \partial \ln k$. The exponent $(z - 2)$ embodies the anomalous scaling between time and space in the critical scaling regime [16]. It follows that $2 - z = -\partial \ln D_k / \partial \ln k$. We emphasize that the previous ansatz (7) should qualitatively well encompass the physics of the model and, moreover, provide accurate estimates of "static" quantities, related to the potential part. However, this level of approximation is not expected to give very accurate dynamical exponents, even less since they are large. Refining these exponents would require to include the field dependence of Z_k and D_k, and as a further step, to enrich the derivative content of (7) [13,17,18].

We can now establish the generic flow equations for reaction-diffusion processes. The flow of V_k is drawn from Eq. (6), evaluated at a uniform and stationary field configuration. After integrating over ω, one gets

$$\partial_k V_k = \frac{1}{2Z_k} \int \frac{d^d p}{(2\pi)^d} \frac{\partial_k R_k}{\sqrt{1 - [\partial_\psi^2 V_k \partial_{\bar{\psi}}^2 V_k / h_k(p)^2]}}, \quad (8)$$

where $h_k(p) = Z_k D_k p^2 + R_k(p) + \partial_{\bar{\psi}\psi}^2 V_k$. The flow of Z_k (D_k) is obtained taking the q^2 (ν) part of the flow of $\partial_{\bar{\psi}, \psi}^2 \Gamma_k(p, \nu)$. These flows depend on the fields, but the resulting exponents should be identical for any field values. However, this property breaks down when any truncation is performed [13]. Since, in the reaction-diffusion models, $\bar{\phi}$ vanishes, and the average of ϕ reaches a uniform and stationary configuration, it is sensible to define the exponents at $\bar{\psi} = 0$ and $\psi(p, \nu) = \psi_{0k}\delta^d(p)\delta(\nu)$. Derivating Eq. (6) twice wrt $\bar{\psi}(-q, -\nu)$ and $\psi(q, \nu)$ yields, after integrating over the internal frequency,

$$\partial_k \partial^2_{\bar\psi\psi}\Gamma_k(q,\nu) = \frac{1}{Z_k}\partial^3_{\bar\psi\psi\psi}V_k\partial^3_{\bar\psi\bar\psi\psi}V_k\int\frac{d^dp}{(2\pi)^d}\frac{\partial_k R_k(p)}{[Z_k i\nu + h_k(p) + h_k(p-q)]^2} - \frac{1}{2Z_k}\partial^2_{\bar\psi\bar\psi}V_k(\partial^3_{\bar\psi\psi\psi}V_k)^2$$

$$\times \int\frac{d^dp}{(2\pi)^d}\partial_k R_k(p)\left(\frac{h_k(p)+h_k(p-q)}{h_k(p)h_k(p-q)[Z_k i\nu + h_k(p)+h_k(p-q)]^2} + \frac{1}{h_k(p)^2[Z_k i\nu + h_k(p) + h_k(p-q)]}\right). \tag{9}$$

As a first step, we show that these equations allow us to recover the universal physics of DP and more precisely to compute the three usually quoted independent critical exponents z, ν, and β. ν describes the scaling behavior of the correlation length near criticality, β that of the order parameter. A field theoretical action $S[\bar\phi,\phi]$ can be derived from the microscopic processes (1)–(3), upon the introduction of two fields, ϕ and $\bar\phi$. After their rescaling and a shift of $\bar\phi$, one gets [14]

$$S[\bar\phi,\phi]\int d^drdt[\bar\phi(\partial_t - D\nabla^2)\phi + (\mu-\sigma)\phi\bar\phi + \sqrt{2\lambda\sigma}(\bar\phi\phi^2 - \phi\bar\phi^2) + \lambda\phi^2\bar\phi^2], \tag{10}$$

which is invariant under the simultaneous changes $\phi(x,t)\to -\bar\phi(x,-t)$ and $\bar\phi(x,t)\to -\phi(x,-t)$. The generic term of the effective potential $V_k(\bar\psi,\psi)$ allowed by this symmetry reads $a_{\alpha\beta}[\psi^\alpha\bar\psi^\beta + (-1)^{\alpha+\beta}\bar\psi^\alpha\psi^\beta]$, which can be expressed in terms of the two invariants $x = \psi\bar\psi$ and $y = \psi - \bar\psi$. Thus V_k can be conveniently parametrized by $U_k(x,y) = V_k(\bar\psi,\psi)$. By numerically integrating the flows (8) and (9), we find that for a fine-tuned initial $(\mu - \sigma)$, corresponding to criticality, the (dimensionless) effective potential flows to a fixed function. The exponents are calculated in the vicinity of this fixed solution. We first implement the well-known local potential approximation (LPA); that is, $Z_k = D_k = 1$. The static exponent ν is very accurate in all dimensions, see Table I, whereas β, deduced from the scaling relation $\beta = 1/2(d + \eta)$, is more imprecise since $\eta = 0$ at this order. We then study the leading order (LO) in derivatives: Z_k and D_k now run with k. The critical exponents are all the

more accurate when η and $(z - 2)$ remain small. They thus deteriorate as the dimension lowers, since η and $(z - 2)$ then become large. As usual with this method, more accurate determinations of η and z rely on a proper description of the momentum and frequency dependence of the two-point correlation function, which would require us to implement a richer ansatz for Γ_k [18], as already emphasized.

We finally come to the most important part of this work: the study of nonuniversal features of the BARW defined by the set of the two processes (1) and (2) ($\mu = 0$). Mean field theory predicts the density to reach a finite saturation value for any positive birthrate σ, and thus the system to be always in the active state. Nevertheless, simulations [20] have brought out the existence of a phase transition in this model in $d = 1$ and $d = 2$, invalidating mean field conclusions. Cardy and Täuber have addressed this question through a field theoretical perturbative study [14] and provided a partial answer relevant for small reaction rates λ/D and σ/D, and in the vicinity of $d = 2$. They have shown that fluctuations can indeed induce, for a nonzero critical birthrate σ_c, a dynamical transition to an absorbing state (belonging to the DP universality class). The underlying reason for the existence of the transition is that the combination of (1) and (2) generates under renormalization the one-particle spontaneous decay (3). This process allows the existence of an absorbing state if its renormalized rate $\mu_R(\sigma,\lambda)$ renders $\mu_R - \sigma_R$ positive [see Eq. (10)]. In $d = 2$, this defines a narrow absorbing region below a critical transition curve given by

$$\sigma_c(\lambda)/D \propto e^{-4\pi D/\lambda}. \tag{11}$$

For $d > 2$, perturbation theory breaks down. However, since the transition curve Eq. (11) is already infinitely flat for small λ/D in $d = 2$, and since fluctuations are expected to be suppressed when the dimension increases, it has been suggested in [14] that no transition should exist in $d = 3$.

We reinvestigate this question using NPRG, which is neither restricted to small λ/D nor to a specific dimension. We can thus explore the phase diagrams of BARW in $d = 2$ and $d = 3$. They are displayed in Fig. 1.

In $d = 2$, we find two regimes. For small λ/D (typically below 4) the transition curve is very accurately fitted by an exponential with a coefficient -11.8, in agreement with Eq. (11) at a 6% level. For large λ/D, $\sigma_c(\lambda)/D$ grows linearly opening up a large absorbing

TABLE I. Critical exponents of DP. (a),(b): NPRG calculations from this work, at the local potential approximation and at leading order. (c) From Monte Carlo simulations [19].

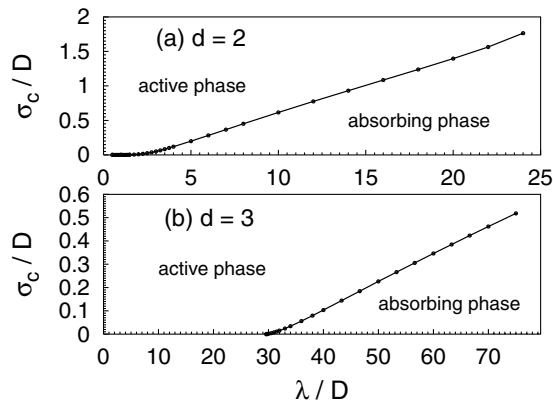| d		(a) LPA	(b) LO	(c) MC
3	ν	0.584	0.548	0.581(5)
	β	0.872	0.782	0.81(1)
	z	0	1.909	1.90(1)
2	ν	0.730	0.623	0.734(4)
	β	0.730	0.597	0.584(4)
	z	0	1.884	1.76(3)
1	ν	1.056	0.888	1.096 854(4)
	β	0.528	0.505	0.276 486(8)
	z	0	1.899	1.580 745(10)

FIG. 1.   Phase diagrams of BARW in $d = 2$ and $d = 3$.

phase. In $d = 3$, we also find two regimes, one with a linear critical curve, and one without transition, separated by a threshold value $\lambda/D \simeq 30$. Let us now give simple arguments highlighting why a transition must exist in $d = 3$, which perturbation theory misses.

When D is large compared with λ and σ, the mechanism of particle destruction is driven by the pair annihilation occurring when wandering particles meet. While in $d = 2$ all the particles can be destroyed through this mechanism, it is not efficient enough to do so in $d = 3$. We thus expect only an active phase at large D in $d = 3$. This corresponds to the result of the perturbation theory, which is indeed valid at small λ/D. On the other hand, in the small D regime where perturbation theory fails, the mechanism of destruction is dominated by "self-destruction"; that is, particles annihilate with their own offspring before they can diffuse. This process no longer requires the random encounter of particles and thus does not depend on the dimension. We therefore expect a transition to occur at small D both in two and three dimensions. These arguments corroborate the phase diagrams obtained from the NPRG analysis. Though, relying on the ansatz (7), we cannot provide a quantitative estimate of the accuracy of the critical rates in Fig. 1, the previous arguments reinforce the NPRG ability to capture the nonuniversal physics of the model over the different diffusive regimes. Moreover, we have performed numerical simulations, which confirm the existence of a DP phase transition in $d = 3$ for large λ/D and hence support our prediction (extensive simulations to quantitatively check the phase diagrams are in progress [21]).

Note that in simulations [20], the implementation of reaction (2) involves the creation of offspring on neighboring sites, contrary to the on-site birth process underlying field theoretical approaches (both [14] and ours). Though this should not alter the behavior of the model

when D is large, it becomes crucial at small D since the "self-destruction" mechanism is then drastically suppressed. This is probably why no transition is found in $d = 3$ in these simulations.

In the present work, we have implemented for the first time NPRG methods in nonequilibrium statistical physics and derived very generic flow equations for reaction-diffusion models. This method has allowed us to recover the universal behavior of directed percolation and moreover to compute the phase diagrams of BARW. We have shown that a phase transition exists in $d = 3$ in these systems contrary to what suggests perturbation theory. The formalism developed here offers an as efficient as promising means of investigation of nonequilibrium physics. This could give some valuable insight into the perennial Kardar-Parisi-Zhang problem, describing roughening transitions in growing interfaces.

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