

Numerical study of a field theory for directed percolation

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A numerical method is devised for the study of stochastic partial differential equations describing directed percolation, the contact process, and other models with a continuous transition to an absorbing state. Owing to the heightened sensitivity to fluctuations attending multiplicative noise in the vicinity of an absorbing state, a useful method requires discretization of the field variable as well as of space and time. When applied to the field theory for directed percolation in $1+1$ dimensions, the method yields critical exponents which compare well against accepted values.

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I. INTRODUCTION

The study of critical phenomena in simple nonequilibrium lattice models has reached the stage where many transitions can be assigned to one of a small set of universality classes. For continuous transitions into an absorbing state, a very high degree of universality has been found, with many examples supporting the prediction [1–3] that such transitions belong generically to the class of directed percolation (DP). Examples include the basic contact process and its variants [4–8], surface reaction models [9,3,10], branching and annihilating random walks with odd parity [11–13], assorted multiparticle processes [14–17], and even models with multiple absorbing configurations [18–22]. Each is an interacting particle system characterized by rules for elementary processes such as creation, annihilation, and diffusion. Looking at the rules, there is little to tell us what sort of critical behavior to expect, nor why it is universal. Understanding of universality emerges instead from the study of coarse-grained formulations which capture the large-scale features essential to critical behavior. In such field theories the microscopic picture of particles on a lattice is replaced by a set of densities which evolve via stochastic partial differential equations (SPDEs). At this level, renormalization-group methods may be applied [1,23–26]. A basis for universality appears if one can show that the continuum descriptions for various models differ only by irrelevant terms. At present, however, there are many more models known (on the basis of numerical work—simulations and/or series analysis) to have DP critical behavior than have been studied using field theory. Useful continuum descriptions of multiparticle processes, for example, have yet to be devised [2,27,28].

It is of interest, therefore, to study SPDEs for nonequilibrium systems and to compare their behavior with the lattice models they are supposed to describe. But solving a nonlinear SPDE is not generally feasible by analytic means and so numerical methods must be sought [30]. Numerical integration has been applied to several SPDEs, for example, the time-dependent Ginzburg-Landau equation describing phase separation [31–33]

and the Kardar-Parisi-Zhang equation [34–36]. In problems with an absorbing state, however, the usual approach does not yield useful results. A method for dealing with such systems is proposed in the present work and is used to study the field theory for the contact process.

The outline is as follows. In Sec. II I describe the original model and the corresponding SPDE. The integration scheme is introduced in Sec. III and results are presented in Sec. IV. A discussion and summary follow in Sec. V.

II. LATTICE MODEL AND FIELD THEORY

In the *contact process* (CP) [4], each site of the d -dimensional cubic lattice \mathbf{Z}^d either is vacant or is occupied by a particle. The transition rules are easily stated: a vacant site with n occupied nearest neighbors becomes occupied at rate $\lambda n/2d$ and particles disappear at a unit rate, independent of their surroundings. Evidently the vacuum is absorbing; the active phase, characterized by a nonzero stationary particle density $\bar{\rho}$, exists only for sufficiently large λ (and only, strictly speaking, in the infinite-volume limit). There is a continuous transition from the vacuum to the active phase at a critical value λ_c [37]. (In one dimension $\lambda_c \simeq 3.2978$ [38,39].) The transition belongs to the universality class of directed percolation. (Note that the d -dimensional CP corresponds to directed percolation in $d+1$ dimensions.)

Janssen [1] proposed a continuum description of the CP and allied models:

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} = a\rho(\mathbf{x}, t) - b\rho^2 - c\rho^3 + \cdots + D\nabla^2\rho + \eta(\mathbf{x}, t). \quad (1)$$

$\rho(\mathbf{x}, t) \geq 0$ is the coarse-grained particle density; the ellipsis represents terms of higher order in ρ . $\eta(\mathbf{x}, t)$ is a Gaussian noise, which respects the absorbing state ($\rho=0$) by virtue of the covariance:

$$\overline{\eta(\mathbf{x}, t)\eta(\mathbf{x}', t')} \propto \rho(\mathbf{x}, t)\delta(\mathbf{x} - \mathbf{x}')\delta(t - t'). \quad (2)$$

This form can be justified by coarse graining the CP, in the limit of large bin size. Let n_i be the number of parti-

cles in bin i and Δn_i the change in this number during a brief interval. The latter has expectation $\overline{\Delta n_i} \propto a n_i + O(n_i^2)$ (with $a \propto \lambda - 1$) and under the customary assumption of Poissonian statistics for reaction systems, its variance equals Δn_i . For sufficiently large bins we may approximate Δn_i by a Gaussian. Thus, since reactions in different bins are uncorrelated, coarse graining the original model leads to a stochastic field theory with Gaussian noise whose autocorrelation is proportional to the local density. (There is also noise due to the fluctuating diffusive current. But diffusive noise does not affect the critical behavior in the present case and so I shall ignore it in the interest of simplicity.) Since Eq. (1) involves multiplicative noise, one must decide upon an interpretation [29]. As shown in Sec. III, the Ito interpretation of Eq. (1) is demanded by physical considerations.

In mean-field approximation [the spatially uniform, noise-free version of Eq. (1)], the vacuum becomes unstable when $a = 0$ and for $a, b > 0$ there is an active state. When fluctuations are taken into account, the critical point shifts to $a_c > 0$ and the critical behavior is nonclassical. For example, the stationary density in the CP scales as $\bar{\rho} \propto (a - a_c)^\beta$, with $\beta \approx 0.277$ in one dimension. (In mean-field theory $\beta = 1$.) Field-theoretic analysis [1,24] reveals that the cubic and higher-order terms are irrelevant to critical behavior as long as $b > 0$. (Such terms are therefore ignored in what follows.) The situation is analogous to that in equilibrium critical phenomena, where the Ising universality class is generic for models with a scalar order parameter and short-range interactions.

Without noise, Eq. (1) is a reaction-diffusion equation, which exhibits a mean-field critical point. It is perhaps surprising that driving a reaction-diffusion equation with multiplicative noise leads to the proper exponents. Of course the condition expressed in Eq. (2) is crucial in this regard. On the other hand, it is not clear whether adding a properly scaled noise to the reaction diffusion equation always yields a useful field theory [2,27].

Further unanswered questions are whether solutions in Eq. (1) exist and, if so, whether they reproduce the phenomenology of the lattice models they are supposed to describe. (For example: Can the field actually fluctuate into the vacuum?) Such issues never arise in renormalization-group analyses, where the SPDE merely serves as a basis for perturbation theory, which proceeds by expanding the formal solution. Since the exponents emerging from the ϵ -expansion analysis of Eq. (1) are in good agreement with series and simulation results, there is no reason to doubt its validity in this context. The present work is concerned with nonperturbative (numerical) solutions to a discretized version of the SPDE.

III. NUMERICAL METHOD

Can Eq. (1) be integrated numerically? To begin, we discretize space, obtaining a set of Langevin equations which in one dimension take the form

$$\frac{d\rho(i,t)}{dt} = a\rho(i,t) - b\rho^2 + D\tilde{\nabla}^2\rho + \eta(i,t), \quad (3)$$

where i is a site index (for convenience we assume a spacing $\Delta x = 1$ in the discretization) and $\tilde{\nabla}^2\rho(i,t) \equiv \rho(i+1,t) + \rho(i-1,t) - 2\rho(i,t)$ is the lattice Laplacian operator. The noise term satisfies $\eta(i,t)\eta(j,t') = \Gamma\rho(i,t)\delta_{i,j}\delta(t-t')$. (Γ is related to the growth rate λ in the CP. We may regard it as constant over the range of parameter values of interest here and set $\Gamma = 1$ from here on). Applying the Cauchy-Euler method to these equations [29], we find

$$\rho(i,t+\Delta t) - \rho(i,t) = [a\rho(i,t) - b\rho(i,t)^2 + D\tilde{\nabla}^2\rho(i,t)]\Delta t + \sqrt{\rho(i,t)\Delta t} Y(i,t), \quad (4)$$

where the $Y(i,t)$ are independent Gaussians with zero mean and unit variance. Equation (4) is similar to the set of stochastic differential equations (SDEs) derived in Ref. [30] from discretization of a SPDE. The latter scheme, however, is not useful here, due to the dominance of the noise in the vicinity of the critical point. Indeed, once we discretize time there is nothing to prevent $\rho(i,t)$ becoming negative. We might attempt to remedy this by stipulating that whenever integration yields $\rho(i,t) < 0$, the density at that site be set to zero. But this artifice is not without drawbacks. We are interested in the critical region, where ρ is small. If the typical magnitude of the first term on the right-hand side is ϵ , the noise term is of order $\sqrt{\epsilon}$ and so overwhelms the deterministic part of the evolution. In the original equation, the cumulative effect of the systematic term is not obliterated by the noise, which has zero mean. But this is no longer so if we truncate the noise in an unsymmetric manner. In simulations using the $\max[\rho, 0]$ rule, the process never reaches the vacuum (even for $a < 0$). Regions of density zero are rapidly repopulated by nearby active sites. It appears, then, that straightforward numerical integration of Eq. (1) is not useful.

Consider, for the moment, the Ito SDE (a Malthus-Verhulst process), with the same local terms as Eq. (1):

$$d\rho = [a\rho - b\rho^2]dt + \sqrt{\rho}d\xi(t), \quad (5)$$

with $\overline{d\xi(t)^2} = dt$. Equation (5) describes Brownian motion in a potential which grows proportional to ρ^3 for large ρ and has a minimum (for $a, b > 0$) at $\rho = a/b$. There is an absorbing boundary at $\rho = 0$, corresponding to the vacuum in the CP. Now suppose we had interpreted Eqs. (1) and (5) as Stratonovich equations. The Ito SDE corresponding to the Stratonovich interpretation of Eq. (5) is [29]

$$d\rho = [a\rho - b\rho^2 + \frac{1}{4}]dt + \sqrt{\rho}d\xi(t). \quad (6)$$

It includes a *constant source term*, so that $\rho = 0$ is no longer absorbing. Clearly this is not the problem we began with. Hence Eqs. (1) and (5) should be taken in the Ito sense.

Integrating Eq. (5) we have

$$\Delta\rho = [a\rho - b\rho^2]\Delta t + \sqrt{\rho}\Delta W, \quad (7)$$

where $\Delta W = \sqrt{\Delta t} Y$ and Y is Gaussian with zero mean and unit variance. Now to prevent $\rho + \Delta\rho$ from going negative, I propose to discretize the density by setting

$\rho = n\rho_{\min}$ ($n \geq 0$) and at the same time to truncate Y symmetrically by restricting its magnitude so that $|Y| \leq Y_{\max}$. We require $Y_{\max} \sqrt{\Delta t} \leq \sqrt{\rho_{\min}}$ to avoid negative densities. This can be achieved in a variety of ways, for example, by setting

$$Y_{\max} = \frac{|\ln \Delta t|}{3} \quad (8)$$

and

$$\rho_{\min} = \frac{(\ln \Delta t)^2 \Delta t}{9}. \quad (9)$$

Equations (8) and (9) represent but one of an infinity of choices. Determining which is optimal for a specific problem is left as a subject for future work. I take $\rho_{\min} \propto \Delta t$ in hopes of minimizing the effect of a discretized density. The relatively slow growth of Y_{\max} poses no essential difficulty. (Note that for $\Delta t = 10^{-4}$ we have $Y_{\max} = 3.07$, about three standard deviations.) Indeed, all noise distributions having zero mean and finite variance should yield qualitatively similar behavior. If one were interested solely in universal properties, the Gaussian could be replaced with a uniform distribution in the interest of computational efficiency.

Having discretized ρ , we can define an integer process by exploiting the invariance of Eq. (5) under the rescaling

$$b \rightarrow b' = ab, \quad (10)$$

$$\rho \rightarrow \rho' = \frac{\rho}{a}, \quad (11)$$

$$\xi \rightarrow \xi' = \frac{\xi}{a}. \quad (12)$$

If we choose $a = \rho_{\min}$, then ρ' is restricted to integers ≥ 0 . Discretization (in time) of Eq. (5) leads to a noise term $Y\sqrt{\rho\Delta t}$; in the rescaled equation it becomes $Y\sqrt{\rho'\Delta t}/a$. (Y is a zero-mean, unit-variance Gaussian, truncated as described above.)

We now have a discretized version of Eq. (5) in which positivity and zero-mean noise are ensured at the cost of a “quantized” density. Since ρ' can change only by integer steps, it is likely (especially for small ρ') that many increments of the density will be rejected for being of less than unit magnitude. It therefore seems advisable to introduce a continuous variable ψ , which accumulates the increments in density at each time step. Whenever $|\psi| \geq 1$, the integer part is transferred to ρ' .

In summary, the numerical scheme for Eq. (5) is as follows. At each time step $\psi \rightarrow \psi + \Delta\psi$, where

$$\Delta\psi = (a\rho' - b'\rho'^2)\Delta t + Y\sqrt{\rho'\Delta t}/a, \quad (13)$$

and

$$\rho' \rightarrow \rho' + [\psi], \quad (14)$$

$$\psi \rightarrow \psi - [\psi], \quad (15)$$

where square brackets denote the integer part. (Initially, ψ is zero.) Equations (13)–(15) may be viewed as a Malthus-Verhulst process in which the population change $\Delta n \equiv \Delta\rho'$ is approximated by a suitably truncated

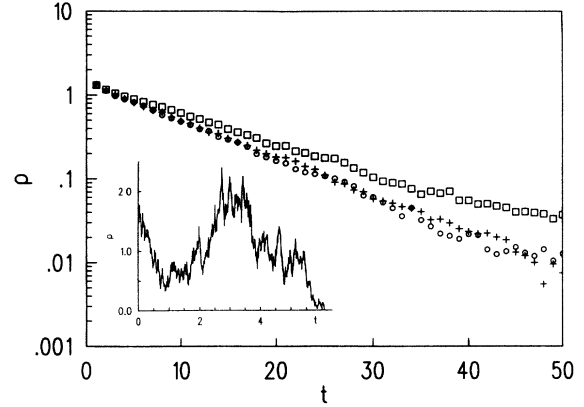


FIG. 1. Evolution of the mean density in the discretized SDE, Eq. (5), for $a=1.5$ and $b=1$. \square , $\Delta t=10^{-3}$; $+$, $\Delta t=2 \times 10^{-4}$; \circ , $\Delta t=10^{-4}$. The inset shows a typical trial ($\Delta t=10^{-3}$).

Gaussian random variable. Simulations show the population fluctuating around a quasisteady value $\rho_{qs} \approx a/b$ and eventually becoming trapped at zero (see the inset of Fig. 1). In Fig. 1 the mean density for a sample of 10^3 trials is plotted for several time increments. (The model parameters are $a=1.5$ and $b=1$; $\rho=1.6$ initially.) The density decays exponentially, with relaxation times 12.9, 9.7, and 9.8 for time increments 10^{-3} , 2×10^{-4} , and 10^{-4} , respectively. This is in good agreement with the mean first passage time 10.3 for hitting $\rho=0$. [The latter is obtained from the Fokker-Planck equation corresponding to Eq. (5) [29].]

Our treatment of the SPDE, Eq. (1), closely parallels that of Eq. (5). Discretization and rescaling of Eq. (3) yields a set of diffusively coupled Malthus-Verhulst processes

$$\Delta\psi_i = (a\rho'_i - b'\rho_i'^2 + D\tilde{\nabla}^2\rho'_i)\Delta t + Y_i\sqrt{\rho'_i\Delta t}/a \quad (16)$$

and

$$\rho'_i \rightarrow \rho'_i + [\psi_i], \quad (17)$$

$$\psi_i \rightarrow \psi_i - [\psi_i]. \quad (18)$$

[The rescaling of Eqs. (10)–(12) does not affect the diffusion coefficient.] We have converted the original SPDE into a lattice of discrete stochastic processes which approaches the continuum model as Δt and $\Delta x \rightarrow 0$.

A final technical point is that when integrating the coupled equations, the three parts of the evolution—deterministic on-site contributions, the noise term, and diffusion—are implemented separately, in turn (over the entire lattice), at each step. (Transfer from ψ to ρ' is made following each of the three substeps.) Unphysical events such as a site becoming empty and subsequently acting as a source for its neighbor, are eliminated by this measure.

IV. RESULTS

I applied the scheme detailed above to systems of several hundred to several thousand sites in order to

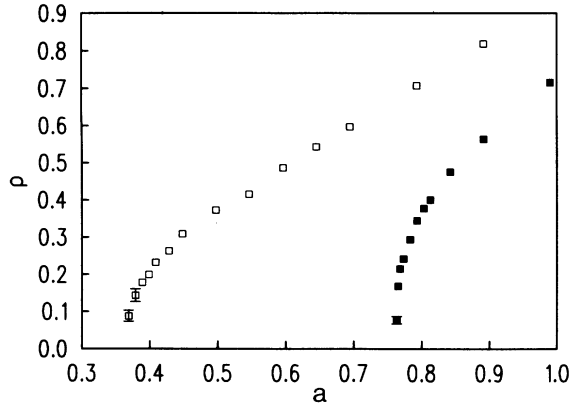


FIG. 2. Steady state density versus a in simulations of the discretized SPDE, Eq. (15), with $b=1$ and $\Delta t=10^{-4}$. Solid squares, $D=1$; open squares, $D=10$.

study the critical behavior of Eq. (1). To begin, I described results for the steady state, obtained in a series of long runs (of duration $t_f \approx 10^4$), on lattices of 500–2000 sites, using a time step $\Delta t=10^{-4}$. The coefficient b was set to unity; diffusion rates $D=1$ and 10 were considered. The stationary density $\bar{\rho}(a)$ (expressed in its original units, prior to rescaling), is shown in Fig. 2. The data suggest a continuous transition to the vacuum at a critical value a_c (≈ 0.77 and 0.36 for $D=1$ and 10, respectively). To estimate the order-parameter exponent β , one must estimate the critical value a_c and then plot the density versus $\Delta = a - a_c$ on log scales. For $D=1$, a reasonably linear plot (for small Δ) is obtained when we choose $a_c=0.769$ (see Fig. 3). A least-squares linear fit to the five points nearest a_c yields a slope $\beta=0.295$, in fair agreement with $\beta=0.277$ for the one-dimensional CP. As is often the case, the slope depends quite sensitively upon one's estimate of the critical point and so this analysis is not very precise. (Taking $a_c=0.765$, for example, one finds $\beta \approx 0.39$.) The slope (≈ 0.45) obtained from the $D=10$ data suggests a more mean-field-like behavior for faster diffusion. Indeed, a_c appears to shift towards

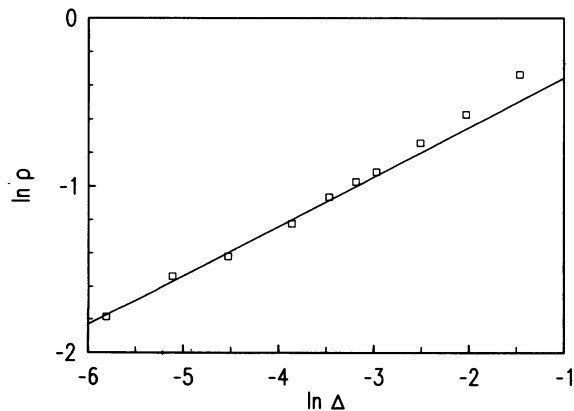


FIG. 3. The data of Fig. 2 ($D=1$) plotted versus $\Delta \equiv a - a_c$, assuming $a_c=0.769$. The straight line, fitted to the five points nearest a_c , has a slope 0.295.

its mean-field 0 with increasing D . For larger D a crossover from mean-field-like to DP-like behavior presumably occurs very near the critical point.

In order to derive quantitative results on critical behavior, I turn to the “time-dependent” method [2,40], in which one studies the dynamics of spreading from a distribution localized near $x=0$. The quantities of interest are the survival probability $P(t)$, mean total density $n(t)$, and mean-square spread $R^2(t)$, for a large sample of independent trials, all with the same initial condition. $P(t)$ denotes the probability of *not* being in the vacuum state at time t , $n(t)$ is the sum of the site densities (averaged over all trials, *including* those which have reached the vacuum by time t), and $R^2(t) \equiv \sum_j j^2 \rho(j,t)/n(t)$. In a subcritical system ($a < a_c$), we expect P and n to decay exponentially, while $R^2(t) \propto t$. For $a > a_c$, P approaches a nonzero limiting value $n(t) \approx t^d$ (in d dimensions) and $R^2(t) \approx t^2$, as a fraction of trials survive indefinitely and spread at finite speed into the surrounding vacuum. At the critical point there is no characteristic time scale for relaxation and the evolution is characterized by nontrivial power laws

$$P(t) \propto t^{-\delta}, \quad (19)$$

$$n(t) \propto t^\eta, \quad (20)$$

and

$$R^2(t) \propto t^z. \quad (21)$$

I studied spreading in simulations beginning with a localized density [typically, $\rho(i,0)=\rho_{\min}$ over the 10–20 sites nearest the origin and $\rho(i,0)=0$ elsewhere) for $D=b=1$. Time increments of 10^{-3} and 10^{-2} were employed, as $\Delta t=10^{-4}$ resulted in excessive run times. The trials (on the order of 10^3 at each a value of interest) ran

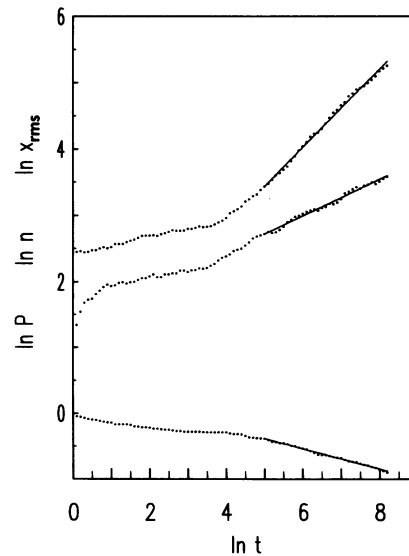


FIG. 4. Time dependence of the survival probability P , total density n , and root-mean-square spread x_{rms} for $a=a_c=0.721$, $b=D=1$, and $\Delta t=10^{-3}$. The straight lines are least-squares fits (for slopes see Table I).

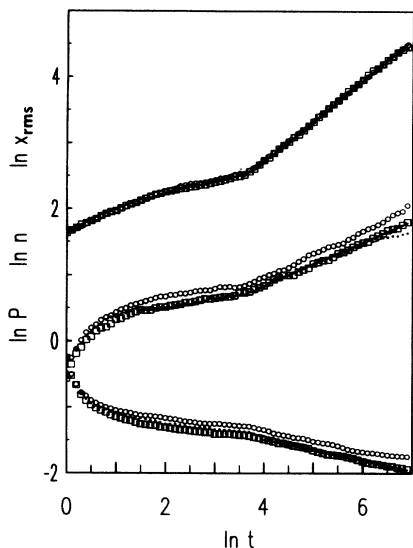


FIG. 5. Same as Fig. 4, but for $\Delta t = 10^{-2}$. Dots, $a = 0.565$; open squares, $a = 0.568$; circles, $a = 0.570$.

to a maximum time of 4000 (1000 in the studies employing $\Delta t = 10^{-2}$) and were performed on lattices of 500–900 sites, sufficiently large that the active region did not reach the boundaries.

Using the criterion of asymptotic power laws at the critical point, I estimate $a_c = 0.7210(5)$ for $\Delta t = 10^{-3}$ and $a_c = 0.568(1)$ for $\Delta t = 10^{-2}$. A plausible explanation for the increase in a_c , as Δt is reduced, is that as ρ_{\min} becomes smaller and the truncation of the noise less severe, fluctuations to zero density occur more readily. When plotted versus $\Delta t^{-1/2}$, the data for a_c suggest a finite limiting value $a_c(0) \approx 0.8$, with $a_c(\Delta t) \approx a_c(0) + \text{const} \times \sqrt{\Delta t}$. The present very limited data (three points for $D = b = 1$) are of course insufficient to permit a firm conclusion in this regard.

Figures 4 and 5 show the evolution of the survival probability, mean population, and root-mean-square spread [$x_{\text{rms}} \equiv \sqrt{R^2(t)}$] for $\Delta t = 10^{-3}$ and 10^{-2} , respectively. In the latter case data from slightly off-critical values are also plotted, which show some curvature. From least-squares fits to the asymptotic linear region in these log-log plots, I derive the exponent estimates listed

TABLE I. Critical exponents from numerical integration of the SPDE.

δ	η	z
	directed percolation	
0.1597(3) ^a	0.317(2) ^b	1.272(7) ^b
	present work $\Delta t = 10^{-3}$	
0.15(1)	0.28(1)	1.18(2)
	present work $\Delta t = 10^{-2}$	
0.159(6)	0.326(10)	1.23(2)

^aReference [38].

^bReference [41].

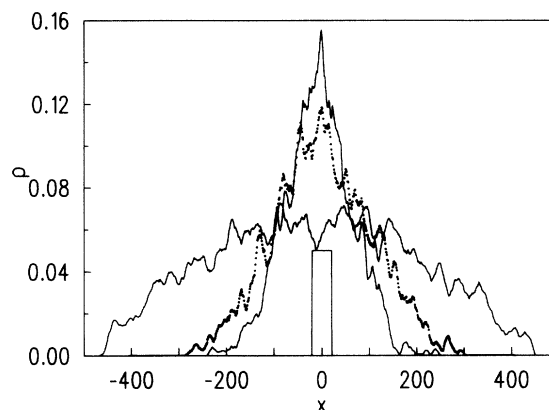


FIG. 6. Average density profiles for $D = B = 1$, $a = a_c = 0.721$, and $\Delta t = 10^{-3}$. From narrowest to broadest: $t = 0, 500, 1000$, and 4000 .

in Table I. Uncertainties, given in parentheses, are subjective estimates based on the spread of exponent values found in simulations with $a \approx a_c$. While not of high precision, the exponents found here compare rather well against the known DP values. Derivation of truly precise results will require longer runs and larger samples, so that a_c can be fixed more reliably, and short-time corrections to scaling can be eliminated by means of a local-slope analysis.

Figure 6 shows the evolution of the mean density profile in the critical system ($\Delta t = 10^{-3}$ and $a = 0.721$). Following an early buildup in the central region, the profile broadens and becomes more sparse. An interesting aspect of the last-time profile, which merits further study, is its large spread, compared to a Gaussian distribution. (That is, $x^4 > 3x^2$.)

V. DISCUSSION

We have seen that some care is required in integrating a field theory with multiplicative noise and an absorbing state. To avoid negative densities and complete dominance of noise, the SPDE must be regularized in some fashion. The present work shows discretization of the field variable to be a suitable method for tempering the equation. Similar conclusions apply to the associated SDE. In fact, the method devised here yields an accurate relaxation time for the latter problem.

Despite discretization of the density, the present approach retains the essential features of a continuum description. The density approximates a continuous variable and spatial coupling occurs solely through diffusion. Moreover, creation and annihilation are expressed here in a naive mean-field-like manner (they are represented, that is, by terms proportional to ρ and ρ^2). Nontrivial critical behavior arises by virtue of properly scaled, multiplicative noise. The exponent values derived from the discretized SPDE are in rather good agreement with accepted values for DP in 1+1 dimensions, arguing for the reliability of the method. The numerical scheme proposed in this work may therefore be of value in testing candidate

theories for models which have so far resisted analysis in continuum representation.

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