Critical behavior of a two-species reaction-diffusion problem

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We present a Monte Carlo study in dimension $d=1$ of the two-species reaction-diffusion process $A+B \to 2B$ and $B \to A$. Below a critical value ρ_c of the conserved total density ρ the system falls into an absorbing state without B particles. Above ρ_c the steady state B particle density $\rho_B^{\rm st}$ is the order parameter. This system is related to directed percolation but in a different universality class identified by Kree *et al.* [Phys. Rev. A **39**, 2214 (1989)]. We present an algorithm that enables us to simulate simultaneously the full range of densities ρ between zero and some maximum density. From finite-size scaling we obtain the steady state exponents $\beta = 0.435(10)$, $\nu = 2.21(5)$, and $\eta = -0.606(4)$ for the order parameter, the correlation length, and the critical correlation function, respectively. Independent simulation indicates that the critical initial increase exponent takes the value $\theta' = 0.30(2)$, in agreement with the theoretical relation $\theta' = -\eta/2$ due to Van Wijland *et al.* [Physica A **251**, 179 (1998)].

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I. INTRODUCTION

We consider a system composed of N particles of two types, A and B, that perform independent random walks on a d-dimensional hypercubic lattice of L sites. The walks arise from jumps between nearest neighbor sites at a transition rate D/a^2, where a is the lattice constant. In the limit of large times and distances D becomes the diffusion constant. At a rate κ each pair of particles (A,B) on the same site reacts according to

$$A+B \to 2B. \tag{1.1}$$

Furthermore a B particle decays into an A particle,

$$B \to A, \tag{1.2}$$

at a rate $1/\tau$. This reaction-diffusion process obviously conserves the total particle number N, and hence the total density $\rho = N/L^d$. We will denote the nonconserved A and B densities by ρ_A and ρ_B, respectively.

Obviously the reactions defined in Eqs. (1.1) and (1.2) amount to postulating a master equation for the time evolution of this system. Since the transition rates do not satisfy detailed balancing with respect to any Hamiltonian, there is no equilibrium state described by a Boltzmann factor. Our interest is in the steady states of this system, and in particular in the stable ones. Let $\rho_A^{\rm st}$ and $\rho_B^{\rm st}$ denote the steady state densities of the A and B particles, respectively. One steady state is the state with only A particles present, that is, with $\rho_B^{\rm st}=0$. If this state is reached, the reaction rules do not allow the system ever to escape from it any more. It is therefore an *absorbing state.* Other steady states, if any exist, must be found as solutions of the time evolution equations.

Whereas this is a difficult problem in general, it is easy to deal with in mean field theory, where ρ_A and ρ_B satisfy the rate equations

$$\frac{\partial \rho_A}{\partial t} = D\Delta\rho_A + \frac{1}{\tau}\rho_B - k\rho_A\rho_B,$$

$$\frac{\partial \rho_B}{\partial t} = D\Delta\rho_B - \frac{1}{\tau}\rho_B + k\rho_A\rho_B \tag{1.3}$$

with $k=\kappa a^d$. The stable steady state solution $(\rho_A^{\rm st},\rho_B^{\rm st})$ of these equations at total density ρ is given by

$$\rho_B^{\rm st} = \begin{cases} 0 & \text{for } \rho \leqslant \rho_c \\ \rho-\rho_c & \text{for } \rho > \rho_c \end{cases} \tag{1.4}$$

and $\rho_A^{\rm st}=\rho-\rho_B^{\rm st}$. Hence the order parameter exponent β, defined in general by

$$\rho_B^{\rm st} \simeq B(\rho-\rho_c)^\beta \text{ as } \rho \to \rho_c^+, \tag{1.5}$$

where B is a constant, here has the mean field value $\beta=1$. Further analysis leads to the mean field values $\nu=1$ and $\eta=0$ for the correlation length and the critical correlation function exponents, respectively. One easily verifies that for $\rho>\rho_c$ the steady state with $\rho_B^{\rm st}=0$ still exists but is unstable.

The process of Eqs. (1.1) and (1.2) is most naturally interpreted as a chemical reaction. Alternatively, Kree, Schaub, and Schmittmann (KSS) [1], who in 1989 were the first to study this process, view it as a model problem in population dynamics with a species B menaced by a polluting substance A. Van Wijland, Oerding, and Hilhorst (WOH) [2] use the same equations to model the propagation and extinction of an epidemic, with the A particles representing healthy individuals and the B particles sick ones. The process of Eq. (1.1) then corresponds to a contamination and that of Eq. (1.2) to spontaneous healing; below we will also occasionally use this terminology. The higher the population density ρ, the more easily the epidemic propagates. The critical density ρ_c is the threshold below which the epidemic becomes extinct.

Phase transitions in steady states fall into universality classes. Three of these are relevant to the present model.

Simpler than our problem, but closely related to it, is the directed percolation (DP) process, which is no doubt the most thoroughly studied one in the field of phase transitions

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into absorbing states. An excellent recent review of DP related work is due to Hinrichsen [3]. The ''DP universality class'' has been shown [4–6] to contain also Schlögl's chemical reaction [7], the contact [6,5,8] or Gribov [9,10] process, and Reggeon field theory [11,5]. All these problems have various equivalent formulations, of which some are convenient for simulations, others more amenable to the methods of exactly soluble lattice models, and still others more suitable for field-theoretical calculations. Their common point is the motion of a *single* species of particles, having interactions that take place upon encounter, whether it be on the same or on adjacent sites; this in addition to possibly allowed spontaneous one-particle creation and/or annihilation.

The process represented by Eqs. (1.1) and (1.2) would reduce to a problem in the DP universality class, with the B particles in the role of the single species, if in some kind of effective medium approximation one were to smear the A's out as a uniform static background. In reality, however, the A particles constitute a dynamical fluctuating environment, coupled to the B's, and this strongly amplifies the B particle density fluctuations. It was shown by KSS [1] that as a consequence the universality class is changed. The reaction-diffusion problem of this paper is in this new ''KSS'' universality class.

In a slightly *generalized* version of the present model, introduced by WOH [2], the A's and B's have unequal diffusion constants D_A and D_B. Those authors showed, in an ϵ expansion, that for $D_B<D_A$ the transition to the absorbing state becomes first order and that for $D_B>D_A$ still another (''WOH'') universality class arises. Monte Carlo simulations of the $D_A\neq D_B$ model were performed in dimension $d=2$ by Leroy *et al.* [12], who focused on the first order transition.

Methods developed over the last two decades, and which have become popular in recent years, allow any stochastic reaction-diffusion process to be cast in the form of a field theory with some action $\mathcal{S}=\mathcal{S}_0+\mathcal{S}_{\rm int}$. Here $\mathcal{S}_0$ is Gaussian and $\mathcal{S}_{\rm int}$ an interaction term that constitutes the model's field-theoretical fingerprint. General methods of passing from the initial definition of a process to its action are described by, e.g., Lee and Cardy [13]. For the particular case of Eqs. (1.1) and (1.2) the action was derived via a Langevin equation by Janssen [14], and from the basic master equation by WOH [2]. It appears that the KSS universality class is characterized by

$$\mathcal{S}_{\rm int}=g\int dx\,dt[\,\psi\overline{\psi}(\psi-\overline{\psi})-\psi\overline{\psi}(\phi+\overline{\phi})\,]. \qquad (1.6)$$

Here g is a coupling constant proportional to the reaction rate k of Eq. (1.1), $\psi(x,t)$ and $\phi(x,t)$ are the fields describing the fluctuations of the B particle and the total particle density, respectively, and $\overline{\psi}(x,t)$ and $\overline{\phi}(x,t)$ are the corresponding conjugate or ''response'' fields. For $\phi=\overline{\phi}=0$ the interaction $\mathcal{S}_{\rm int}$ of Eq. (1.6) reduces to that of directed percolation.

The field-theoretical formulation allows the techniques of the renormalization group to be applied. Dimensional analysis shows that the upper critical dimension is $d_c=4$. KSS [1] found the leading order of the ϵ expansion of the critical exponents in dimension $4-\epsilon$,

$$\beta=1-\frac{\epsilon}{32},\quad \nu=\frac{1}{2}+\frac{\epsilon}{8},\quad \eta=-\frac{\epsilon}{8}. \qquad (1.7)$$

These contrast with the DP exponents, which to lowest order in ϵ read $\beta_{\rm DP}=1-\frac{1}{6}\epsilon$, $\nu_{\rm DP}=\frac{1}{2}+\frac{1}{16}\epsilon$, and $\eta_{\rm DP}=-\frac{1}{6}\epsilon$. We recall [1] that in steady states, as opposed to equilibrium states, the correlation function $g(r)$ at criticality decays with distance r as $g(r)\sim 1/r^{d+\eta}$ and that the exponents satisfy the relation $2\beta=\nu(d+\eta)$.

It is our purpose to perform an accurate determination of the critical exponents in dimension $d=1$ of the KSS universality class. We compare our results to their analogs in the $d=1$ DP universality class, and to the ϵ expansion of the KSS class. The WOH class is beyond the aim of the present study.

II. SIMULATION IN ONE DIMENSION

A. Simulation rules

We consider a one-dimensional lattice of L sites with periodic boundary conditions and lattice constant $a=1$, occupied by N independently moving particles. Time is discretized into steps $t=0,1,2,\ldots$. Each time step consists of the successive application of three rules.

(1) Diffusion rule. Each particle has the possibilities (i) to stay on its site, (ii) to move to its right neighboring site, or (iii) to move to its left neighboring site, each with probability $\frac{1}{3}$. This amounts to choosing the diffusion constant equal to $D=\frac{1}{3}$.

(2) Healing rule. Each B particle is converted into an A particle with ''healing probability'' $p_H=1-e^{-1/\tau}$, where τ is the average healing time. In the simulations we took $\tau=30$, so that $p_H=0.032\,78\ldots$.

(3) Contamination rule. When a site is occupied by one or more B particles, then all A's that may be present additionally on that site are turned into B's with probability 1.

These rules fully determine the simulation procedure. They imply that at the end of any time step any nonempty lattice site contains only *one* type of particle: either A's or B's (and hence it is possible to speak of the type, A or B, of a *site* at any instant of time). For consistency the initial state should also obey this condition.

B. Algorithm

The simulation data at the basis of the theoretical analysis (see Sec. II C) will consist of ρ_B versus ρ curves at various system sizes L. At fixed L, due to our time saving algorithm, there is no need for a whole series of simulations at successive particle densities $\rho=\rho_1,\rho_2,\ldots$. Instead we are able to consider, in a single simulation with N particles, *simultaneously* the full range of particle densities $\rho=0,1/L,2/L,3/L,\ldots,(N-1)/L,N/L$. We describe first the idea at the basis of this algorithm, and then its precise mathematical implementation.

1. Relating systems with different particle numbers

The particle trajectories are mutually independent. Along its trajectory a particle will change its type (from A to B and vice versa) by alternating events of contamination and heal-

ing. Its trajectory is, however, also *independent* of its instantaneous type, since A's and B's move in exactly the same way. Let us call the trajectory of the jth particle, together with the information about its type at each instant of time, the jth ''world line.''

From n to n+1 particles. Let us now do a thought experiment (we call it this because the actual algorithm is implemented differently). Suppose that the simulation of an n-particle system on a lattice of size L, during a time interval T, has produced a collection of n world lines indexed by $j=1,2,\ldots,n$. We can then construct, without redoing a full new simulation, the collection of world lines for a simulation—strongly correlated to the first one—with one extra particle, the $(n+1)$th. This is done as follows.

(i) Choose the initial position and type of the $(n+1)$th particle.

(ii) Determine by Monte Carlo simulation its trajectory in the time interval $1,2,\ldots,T$, independently of the n trajectories already known.

(iii) Determine the effect of the type of this new particle on the types of all the other particles; that is, apply the following rules: (a) the new particle, when of type A, will become a B when arriving on a site with one or more B's present, in accordance with the contamination rule (3) above; (b) the new particle, when of type B, will spontaneously heal (become an A) with probability p_H at each time step in accordance with the healing rule (2) above; and, until healthy, it will contaminate any of the n original particles that it meets; (c) an original particle thus contaminated will continue along its known trajectory, but now has to be subjected itself also at each time step to the healing rule; it may contaminate in turn other particles, etc.

So the introduction of the new particle creates an avalanche of new contaminations (which may either die out or else will finally affect the entire system). This completes the thought experiment in which we construct $n+1$ world lines from n.

It is important to observe that this construction leaves the n original trajectories as they are, but changes only along certain parts of them the associated particle type from A to B. No inverse changes (from B to A) occur. The full information of *both* the original n-particle simulation *and* the new $(n+1)$-particle simulation may be compactly represented by (i) the $n+1$ indexed trajectories of the $(n+1)$-particle simulation, with the rule that those of indices $1,2,\ldots,n$ make up the trajectories of the n-particle system; (ii) $n+1$ symbolic ''type labels'' μ_j such that, for $j=1,\ldots,n$,

$\mu_j=B_{n+1}B_n$ if particle j is of type B in both simulations,

$\mu_j=B_{n+1}A_n$ if particle j is of type B in the $n+1$ particle simulation, but of type A in the n particle simulation,

$\mu_j=A_{n+1}A_n$ if particle j is of type A in both simulations,

and furthermore for $j=n+1$ [recall that the $(n+1)$th particle was absent in the n-particle simulation]

$\mu_{n+1}=B_{n+1}0_n$ if particle $n+1$ is of type B in the $n+1$ particle simulation,

$\mu_{n+1}=A_{n+1}0_n$ if particle $n+1$ is of type A in the $n+1$ particle simulation,

which exhausts all possibilities for the particle types. We emphasize that the μ_j are time step dependent.

From 0 to N particles. By iteration we may construct from a collection of $n+1$ world lines one of $n+2$ world lines, etc. At each iteration step the number of possibilities for the labels μ_j increases.

Let us now start from a 0-particle system and iteratively construct the collections of world lines of systems having, successively, $0,1,2,\ldots,N',\ldots,N$ particles. The different possibilities for the type of the jth particle may be distinguished by a label μ_j, itself characterized by an integer ν_j. We indicate by

$$\mu_j=B_NB_{N-1}\cdots B_{\nu_j}A_{\nu_j-1}\cdots A_j0_{j-1}\cdots 0_10_0 \quad (2.1)$$

that particle j is of type A in the systems with $N'=j,j+1,\ldots,\nu_j-1$ particles; of type B in the systems with $N'=\nu_j,\ldots,N$ particles; and absent in systems with only $N'=0,1,\ldots,j-1$ particles. Here ν_j ranges through $\nu_j=j,j+1,\ldots,N+1$, which gives $N-j+2$ possibilities. The special values $\nu_j=N+1$ ($\nu_j=j$) correspond to particle j being of type A (of type B) for all $N'=j,j+1,\ldots,N$. Clearly the string of symbols on the right-hand side (RHS) of Eq. (2.1) is entirely determined by the integers j and ν_j. We will refer to ν_j as the *type number* of particle j. Hence the full information on the world lines of the whole sequence of $0,1,2,\ldots,N$ particle systems is contained in (i) the N trajectories indexed by $j=1,2,\ldots,N$, with the rule that those of indices $1,2,\ldots,N'$ make up the trajectories of the N' particle system; (ii) for each j, at each instant of time, the type number ν_j. Below we show that there exists an algorithm that generates this full information sequentially in time and, in fact, as a Markov process.

2. Implementation of the algorithm

The mathematical rules of the algorithm are quite simple to state. They require, moreover, very little extra programming effort with respect to a standard algorithm.

Algorithm. N random walk trajectories indexed by $j=1,2,\ldots,N$ are generated in the standard way. The jth particle carries a type number ν_j, which is an integer that may take the values $\nu_j=j,j+1,\ldots,N+1$. The simulation rules of Sec. II A translate into two operations on the ν_j.

(a) At any time step at which $\nu_j<N+1$, particle j is subjected to the healing rule; if healing is not successful ν_j remains unchanged, but if it is successful we replace

$$\nu_j\mapsto N+1. \quad (2.2)$$

(b) The contamination rule implies that for any site occupied by $r\geq 2$ particles $j_1,\ldots,j_s,\ldots,j_r$ we have to carry out the replacements

$$\nu_{j_s}\mapsto \max(j_s,\min(\nu_{j_1},\ldots,\nu_{j_r})) \quad \text{for } s=1,\ldots,r. \quad (2.3)$$

This completes the description of the algorithm.

At any time during the simulation one may take data on any N'-particle system with $0\leq N'\leq N$ by interpreting the ν_j according to the scheme

$$\text{particle } j \text{ is} \begin{cases} \text{absent} & \text{for } N'+1 \leqslant j \leqslant N \\ \text{present and of type } A & \text{for } 1 \leqslant j \leqslant N' \text{ and } N'+1 \leqslant \nu_j \leqslant N+1 \\ \text{present and of type } B & \text{for } 1 \leqslant j \leqslant N' \text{ and } j \leqslant \nu_j \leqslant N'. \end{cases} \tag{2.4}$$

The three conditions corresponding to the three possibilities in the above equation may be read either as restrictions on N' at given j and ν_j or as restrictions on j and ν_j at given N'.

Mathematical proof. Choose an arbitrary $N' \in \{1, \ldots, N\}$. According to Eq. (2.4) above this divides the particles into those indexed by $j = N'+1, \ldots, N$, which are ''absent,'' and the remaining ones, which are ''present.'' We prove now that the N' world lines of the particles present are the result of a faithful execution of the original simulation rules stated in Sec. II A. As far as the trajectories go, this is evident. It remains to consider *(a)* healing and *(b)* contamination. The index $i = 1, \ldots, N'$ will denote a particle present. The scheme (2.4) has to be borne in mind throughout.

(a) If a particle i is of type B, then it has $\nu_i \leqslant N'$, so certainly $\nu_i \leqslant N$, and the algorithm described above subjects it to the healing rule in the same way as prescribed by the original algorithm of Sec. II A. There is no need to worry about the fact that the algorithm also subjects some of the A particles present to the healing rule; for any outcome they remain of type A.

(b) Suppose that at a certain time, on a certain site, $i \in \{j_1, \ldots, j_s, \ldots, j_r\}$, that is, particle i is among r particles (out of the full set of N) that meet on that site. Suppose moreover that i is of type A, that is, it has $\nu_i \geqslant N'+1$. We ask now under what conditions this particle i can be contaminated, that is, acquire a value ν_i less than $N'+1$. Equation (2.3) shows that for that to happen we need both $i \leqslant N'$ and $\min(\nu_{j_1}, \ldots, \nu_{j_r}) \leqslant N'$. The first condition is automatically satisfied. For the second condition to be satisfied it is necessary and sufficient that at least one of the other particles on the site in question have $\nu_{j_s} \leqslant N'$. Now for any $k \in \{j_1, \ldots, j_r\}$ corresponding to an absent particle we have $k \geqslant N'+1$, whence $\nu_k \geqslant N'+1$, and therefore if the second condition is to be fulfilled, this can be due only to one of the particles present. The interpretation of this is that contamination occurs if and only if at least one other particle present is of type B, exactly as prescribed by the original algorithm of Sec. II A. This completes the proof that for any N' the present algorithm is equivalent to the original one.

Further comments. The algorithm is not limited to dimension $d=1$. It is essential, however, that the diffusion constants of the two particle types be equal. Variants of the algorithm are easily imagined. For example, we may simulate this model also at fixed particle number N but simultaneously for the full continuum of healing times $0 < \tau < \tau_{\max}$. In this case the heuristic discussion relates two systems with healing times τ and $\tau + \Delta\tau$, and in the actual implementation each particle j carries a real label τ_j with an interpretation analogous to that of the ν_j. We do not pursue this idea any further here.

C. Finite-size scaling

1. Finite-size effects

The critical point ρ_c and the nontrivial stable steady state with $\rho_B^{\rm st} > 0$ are well defined only in the limit $L \to \infty$. At finite L and for ρ sufficiently above ρ_c, there appears a long-lived metastable state instead. In this state, typically, as a function of time, $\rho_B(t)$ will fluctuate around a plateau value $\tilde{\rho}_B$ for a very long time, until by an accidental fluctuation all B particles disappear and the system enters irreversibly into the absorbing state. For smaller L and/or for $\rho \lesssim \rho_c$ an initially nonzero B particle density fluctuates wildly in the course of time until it vanishes. We will first extend the notion of plateau value to this regime of L and ρ.

Let $\mathbf{n}$ be the set of phase space variables and $P(\mathbf{n},t)$ their probability distribution. For any finite L this distribution will eventually contract onto the absorbing state with $\rho_B^{\rm st} = 0$. Let $P_+(\mathbf{n},t)$ be the decaying probability distribution on the rest of phase space. For large times t we expect

$$P_+(\mathbf{n},t) \sim e^{-t/T_L(\rho)} \tilde{P}(\mathbf{n}) \quad (t \to \infty), \tag{2.5}$$

where $\tilde{P}(\mathbf{n})$ is the slowest decaying mode and $T_L(\rho)$ its decay time. In the limit $L \to \infty$ and for $\rho > \rho_c$ this decay time tends to infinity and $\tilde{P}$ becomes the probability distribution of the nontrivial steady state. We define now $\tilde{\rho}_B(\rho, L)$ as the density of B particles averaged with respect to $\tilde{P}$. We expect that

$$\lim_{L \to \infty} \tilde{\rho}_B(\rho, L) = \rho_B^{\rm st} \tag{2.6}$$

with $\rho_B^{\rm st}$ given by Eq. (1.5) for $\rho \to \rho_c^+$ and equal to zero for $\rho \leqslant \rho_c$.

2. Finite-size scaling

We apply to the averages calculated with respect to $\tilde{P}$ the usual scaling hypotheses for equilibrium states. We assume that $\tilde{\rho}_B$ satisfies the finite-size scaling law

$$\tilde{\rho}_B(\rho, L) \simeq C L^{-\beta/\nu} F(L \delta\rho^{\nu}) \tag{2.7}$$

valid for $\delta\rho \equiv \rho - \rho_c$ sufficiently small and L sufficiently large; here C is a constant and F a scaling function that may be normalized to $F(0) = 1$ and should satisfy $F(x) \sim x^{\beta/\nu}$ as $x \to \infty$ to ensure the consistency of Eqs. (2.7) and (2.6) as $\delta\rho \to 0^+$. It follows that at the critical point $\rho = \rho_c$ one has $\tilde{\rho}_B(\rho_c, L) \simeq C L^{\beta/\nu}$. The preceding properties imply that the ratios

$$R_{2L,L}(\rho) = \frac{\tilde{\rho}_B(\rho, 2L)}{\tilde{\rho}_B(\rho, L)}, \tag{2.8}$$

TABLE I. System size L, measuring interval (T_1, T_2), and number of runs R_L.

L	T_1	T_2	R_L
25	500	1 000	8×10^6
50	1 000	2 000	4×10^6
100	1 500	5 000	10^6
200	20 000	60 000	9×10^4
400	50 000	100 000	16×10^3

when drawn as functions of ρ for different L, should all intersect in the single point $(\rho_c, 2^{-\beta/\nu})$.

III. RESULTS

A. Steady state exponents β, η, ν

1. Determination of ρ_c and β/ν

The practical determination of averages with respect to $\widetilde{P}$ requires the following considerations. Let us consider a large number of runs (realizations of the stochastic process defined in Sec. II A). Then $\widetilde{P}$ is the distribution of all systems that have survived (that is, have not entered the absorbing state) at time t, in the limit $t\to\infty$. The problem is that in this limit the fraction of surviving systems tends to zero. Hence in practice a compromise is needed. Initially all particles were taken to be B's. At given L we determined $\widetilde{\rho}_B$ by averaging $\rho_B(t)$ on an interval $T_1 \leqslant t \leqslant T_2$ with T_1 large enough to eliminate transient effects due to the particular initial state, and T_2 not too large compared to the decay time $T_L(\rho)$. Table I shows the system sizes L that we considered, the intervals (T_1, T_2) used to collect data, and the numbers R_L of independent runs carried out. We have adhered to the common idea that in finite-size scaling it is better to work with not too large system sizes and use the available computer time to increase the accuracy of the data, in our case by augmenting R_L.

In Fig. 1 we show $\widetilde{\rho}_B$ so obtained as a function of ρ for $L=25,50,100,200,400$. The squares represent the data points

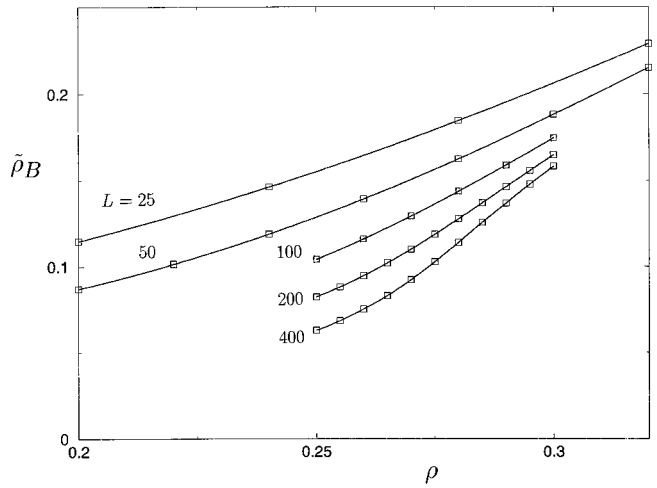

FIG. 1. B particle density $\widetilde{\rho}_B$ (see text) in systems of different sizes L as a function of the total particle density ρ.

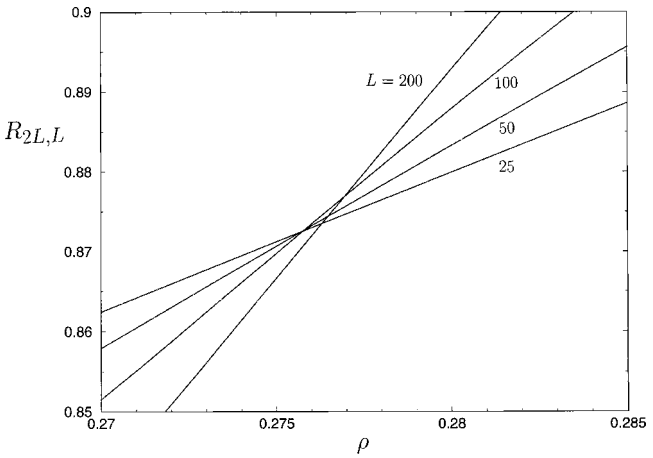

FIG. 2. Ratios $R_{2L,L}$ defined in Eq. (2.8) for various system sizes L as a function of the total particle denstity ρ.

and the curves were obtained by spline interpolation. The statistical error bars in the data points are of the order of 0.01% for $L=25,50,100$ and of the order of 0.1% for $L=200,400$. Curves with different L result from independent simulations and are uncorrelated. Due to the algorithm of Sec. II B statistical errors in neighboring data points with the same L are correlated; it is safest to assume that they are affected by the same error. Figure 2 shows the ratios $R_{50,25}$, $R_{100,50}$, $R_{200,100}$, and $R_{400,200}$ as a function of ρ, and we have expanded the region of the intersection points. The statistical error is about ±0.001 for $R_{50,25}$ and $R_{100,50}$ and about ±0.01 for $R_{200,100}$ and $R_{400,200}$. Because of this we believe that the near coincidence of the three intersection points of the first three curves is somewhat fortuitous (upon magnification they resolve into three distinct intersections). Our estimate of the coordinates of the intersection point $(\rho_c, 2^{-\beta/\nu})$ is $\rho_c = 0.2757\pm0.0010$ and $2^{-\beta/\nu}=0.8725\pm0.0010$. These error bars do not take into account any possible systematic errors that might be inherent in our procedure. With this proviso, it follows that $\beta/\nu=0.197\pm0.002$.

2. Determination of β

We now proceed to determine ν and β separately. Knowing the critical point ρ_c, we determine the best fit of the data compatible with the power law of Eq. (1.4). Since we do not have direct data for the infinite-volume quantity $\rho_B^{\rm st} = \widetilde{\rho}_B(\rho,\infty)$, we first extrapolate $\widetilde{\rho}_B(\rho,L)$ to the $L=\infty$ limit and then fit the power law to the extrapolated data. The extrapolation may be performed fairly accurately in the density regime $\rho \gtrsim 0.3$, away from the critical point, where the problem of slow relaxation is much less severe and we were able to consider system sizes $L=400$, 800, 1600, and 3200. Figure 3 shows $\widetilde{\rho}_B(\rho,L)$ as a function of L for $\rho=0.305$–0.330. The simulation data, represented by the open squares, exhibit the expected $O(1/L)$ finite size effect. The closed squares at $L=\infty$ are the extrapolation results. Statistical errors range from much smaller than the symbols when $\rho=0.330$ to roughly the size of the symbols when $\rho=0.305$. For $\rho\leqslant0.300$ extrapolation of the data seemed too uncertain and was not attempted. By fitting the extrapolated values to Eq. (1.5) with $\rho_c=0.2757$ we arrive at the estimate

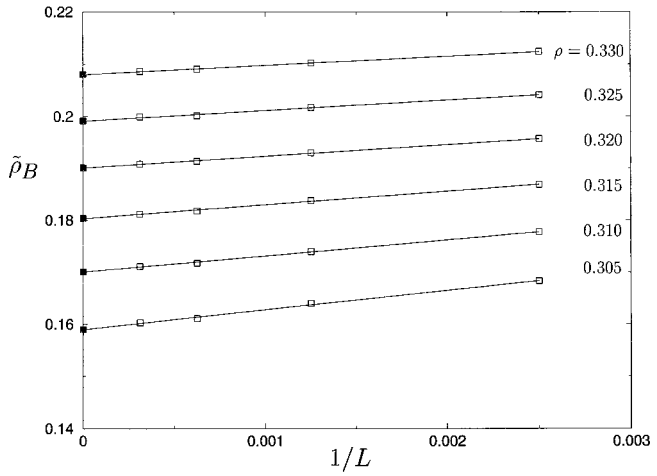

FIG. 3. B particle density $\tilde{\rho}_B$ as a function of inverse system size L^{-1} for various densities ρ above the critical density $\rho_c = 0.2757$. The open squares are measured values, the straight lines are best linear fits, and the closed squares result from extrapolation. The extrapolated values serve to determine β.

$\beta = 0.435 \pm 0.010$. The uncertainties in β are mainly due to the uncertainty in the value of ρ_c. Employing again the exponent relation $1 + \eta = 2\beta/\nu$ we arrive at our final estimates,

$$\beta = 0.435 \pm 0.010, \quad \nu = 2.21 \pm 0.05, \quad \eta = -0.606 \pm 0.004. \tag{3.1}$$

These exponent values show that the ϵ expansion of Eq. (1.7), unsurprisingly, becomes highly inaccurate when the dimension goes down as far as $d = 1$. They may also be compared to the analogous exponents in the $d = 1$ DP universality class. These are known with an impressive numerical accuracy (based on low density series expansions by Jensen [15]) and take the values $\beta_{\mathrm{DP}} = 0.276\,486\,(8)$, $\nu_{\mathrm{DP}} = 1.096\,854\,(4)$, and, via the exponent relation given above, $\eta_{\mathrm{DP}} = -0.495\,86\,(2)$. The difference between the DP and the KSS universality classes, which starts to appear when the spatial dimension d falls below its upper critical value $d_c = 4$, has become very large indeed in dimension $d = 1$.

3. Algorithmic efficiency

Updating the type numbers ν_j costs only very little extra time compared to a standard algorithm. Since at fixed system size L all densities are simulated simultaneously, the gain with respect to a standard algorithm is roughly a factor equal to the number of density points required. This, however, overestimates the efficiency when the different density points require very different run lengths and/or numbers of runs (i.e., different values of the quantities denoted, respectively, by T_2 and R_L in Table I), in which case the actual run must have the largest of those T_2 and R_L and the efficiency of the algorithm is reduced. In our case the actual gain in simulation time has been a factor of around 10.

B. Critical initial increase exponent θ'

Precisely *at* the critical point of a continuous phase transition the stationary value of the order parameter is zero. *Critical initial increase* is the phenomenon that at that point an initially nonzero order parameter will first rise with time as a power law $t^{\theta'}$, pass through a maximum at some time $t = t_{\max}$, and only then start its final decay to zero. Here θ' is the *critical initial increase* exponent (called simply θ by some authors). This phenomenon, first pointed out and explained theoretically in 1989 by Janssen, Schaub, and Schmittmann [16] (see also Diehl and Ritschel [17]), has since been discovered in Monte Carlo simulations by many authors (see, e.g., Li, Ritschel, and Zheng [18], Li, Schülke, and Zheng [19], Grassberger [20], and Ritschel and Czerner [21], who all deal with the Ising model near criticality). The exponent θ' is observable in a time regime $t_{\mathrm{micr}} \ll t \ll t_{\max}$, where t_{micr} is the microscopic time scale and where $t_{\max} \to \infty$ when the initial order parameter goes to zero and the system size to infinity.

When these ideas are applied to the reaction-diffusion problem of this work, we are led to expect [2] that at $\rho = \rho_c$ a small positive $\rho_B(0)$ will initially increase as

$$\rho_B(t) \sim \rho_B(0) t^{\theta'}. \tag{3.2}$$

In the general case θ' is not related in any known way to the other exponents of the problem. Theoretical work by WOH [2] has shown that for the DP and KSS universality classes the relation

$$\theta' = -\frac{\eta}{z} \tag{3.3}$$

must hold. The dynamical critical exponent z that occurs here is for the KSS class given [1,2] by the mean field value $z = 2$ in all dimensions d, so that for $d = 4 - \epsilon$ we have from Eqs. (3.3) and (1.7) that to linear order $\theta' = \frac{1}{16}\epsilon$. The DP exponent z_{DP} has a nontrivial dimensional dependence which to linear order in ϵ leads [2] to $\theta'_{\mathrm{DP}} = \frac{1}{12}\epsilon$. In dimension $d = 1$ the value of η found in the preceding section together with Eq. (3.3) implies the numerical value $\theta' = 0.303 \pm 0.002$.

We present here the first Monte Carlo observation to our knowledge of critical initial increase in a steady state, i.e., in a system that does not have a Boltzmann equilibrium. We considered systems of size $L = 127,254,508,1016$ with $N = 35,70,140,280$ particles, respectively, and hence having a density $\rho = 0.275\,59\ldots$ almost identical to the value of ρ_c determined above. Each system was started in a state with a single B particle. Figure 4 shows the initial rise with time of the normalized order parameter $\rho_B(t)/\rho_B(0)$, obtained as an average over 10 000 runs for the sizes $L = 127,254,512$, and over 20 000 for $L = 1016$. The dashed line is the theoretically expected straight line with slope equal to the Monte Carlo value of $\theta' = 0.303$ found in the preceding section. For the smaller system sizes the order parameter passes through a maximum inside the measuring time interval; for the larger system sizes only the initial increase is seen.

In order to estimate θ' from these curves let us now consider the one for $L = 1016$. In view of the value $\tau = 30$ of the single particle healing time (see Sec. II A), the time regime $t \lesssim 100$ should certainly be considered as microscopic and unsuitable for extracting θ', even though it is not clear exactly where the microscopic regime ends. For $t \gtrsim 10\,000$ the order parameter rises more and more slowly under the influence of the approaching maximum. From the condition

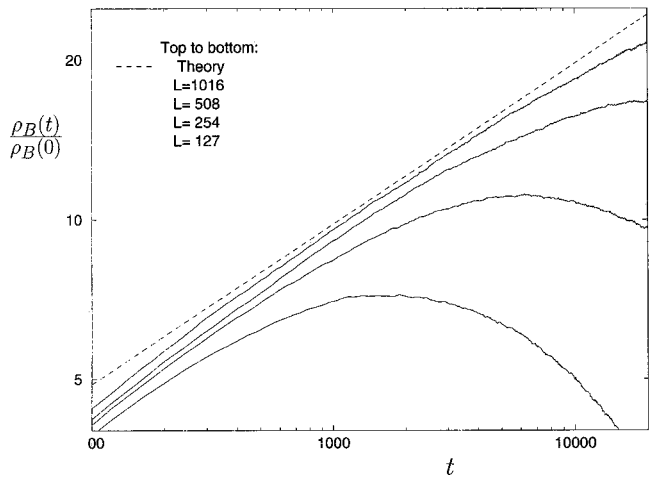

FIG. 4. Initial increase of the density $\rho_B(t)$ from a starting configuration with a single B particle in systems of various sizes L at total density $\rho \approx \rho_c$. The straight line represents the theoretical power law with the exponent $\theta' = 0.303$ determined in Sec. II.

$t_{\mathrm{micr}} \ll t \ll t_{\mathrm{max}}$ we may conclude that in the present case θ' should be extracted from a time regime such that $100 \ll t \ll 10\,000$. The best fit of θ' decreases from $\theta' = 0.317$ in the interval $500 < t < 800$ to $\theta' = 0.288$ for $1500 < t < 2400$. This leads us to the independent estimate $\theta' = 0.30 \pm 0.02$, less precise than, but in full agreement with, the value $\theta' = 0.303$ deduced from the static measurements in Sec. II.

A comparison with the DP universality class is again interesting. This class has [3] for the corresponding $d = 1$ exponent $\theta'_{\mathrm{DP}} = 0.313\,686\,(8)$. Although the KSS and DP values are numerically close, the ϵ expansion provides a strong argument that they are nevertheless different.

IV. CONCLUSION

We have made Monte Carlo estimates of the critical exponents in dimension $d = 1$ of one of the simplest paradigms of steady state reaction-diffusion systems, representative of the KSS universality class, which is closely related to, but distinct from, the directed percolation universality class. The values of the static exponents β, ν, and η were estimated after an independent determination of the critical point via finite-size scaling. The uncertainties in the final values are mainly due to the uncertainty in locating the critical point. The critical initial increase exponent θ' may then be obtained from the theoretical scaling law (3.3) derived for this system by WOH [2]. Independent time dependent simulations performed at the critical point show agreement with this value and hence confirm that scaling law.

It is interesting to note that the simple fractions

$$\beta = \tfrac{4}{9}, \quad \nu = \tfrac{20}{9}, \quad \eta = -\tfrac{3}{5}, \quad \theta' = \tfrac{3}{10} \tag{4.1}$$

are consistent with the data of this work. There is, however, no compelling reason why the exponents of this nonconformal system should be rationals. Rational values conjectured [22] at one time for the DP universality class had to be abandoned later (see, e.g., [15]) after higher precision numerics were obtained.

We have compared our results to the analogous values of the DP exponents in dimension $d = 1$ and to the ϵ expansions of both the KSS and DP classes. It is interesting to observe that the four inequalities $\beta > \beta_{\mathrm{DP}}$, $\nu > \nu_{\mathrm{DP}}$, $\eta > \eta_{\mathrm{DP}}$, and $\theta' < \theta'_{\mathrm{DP}}$, known to hold analytically in the ϵ expansion, continue to be satisfied numerically in dimension $d = 1$.

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[1] R. Kree, B. Schaub, and B. Schmittmann, Phys. Rev. A **39**, 2214 (1989).
[2] F. van Wijland, K. Oerding, and H. J. Hilhorst, Physica A **251**, 179 (1998).
[3] H. Hinrichsen, eprint cond-mat/0001070.
[4] P. Grassberger and A. de la Torre, Ann. Phys. (N.Y.) **122**, 373 (1979).
[5] P. Grassberger and K. Sundermeyer, Phys. Lett. **77B**, 220 (1978).
[6] J. L. Cardy and R. L. Sugar, J. Phys. A **13**, L423 (1980).
[7] F. Schlögl, Z. Phys. **253**, 147 (1972).
[8] S. P. Obukhov, Physica A **101**, 145 (1980).
[9] V. N. Gribov, Zh. Éksp. Teor. Fiz. **53**, 644 (1967) [Sov. Phys. JETP **26**, 414 (1968)].
[10] V. N. Gribov and A. A. Migdal, Zh. Éksp. Teor. Fiz. **55**, 1498 (1968) [Sov. Phys. JETP **28**, 784 (1969)].
[11] M. Moshe, Phys. Rep., Phys. Lett. **37C**, 255 (1978).
[12] J.-P. Leroy, H. J. Hilhorst, K. Oerding, and F. van Wijland, (unpublished).
[13] B. P. Lee and J. L. Cardy, J. Stat. Phys. **80**, 871 (1995).
[14] H. K. Janssen, Z. Phys. B: Condens. Matter **23**, 151 (1981).
[15] I. Jensen, J. Phys. A **32**, 5233 (1999).
[16] H. K. Janssen, B. Schaub, and B. Schmittmann, Z. Phys. B: Condens. Matter **73**, 539 (1989).
[17] H. W. Diehl and U. Ritschel, J. Stat. Phys. **73**, 1 (1993).
[18] Z.-B. Li, U. Ritschel, and B. Zheng, J. Phys. A **27**, L837 (1994).
[19] Z.-B. Li, L. Schülke, and B. Zheng, Phys. Rev. Lett. **74**, 3396 (1995); Phys. Rev. E **53**, 2940 (1996).
[20] P. Grassberger, Physica A **214**, 547 (1995).
[21] U. Ritschel and P. Czerner, Phys. Rev. E **55**, 3958 (1997).
[22] J. W. Essam, A. J. Guttmann, and K. De'Bell, J. Phys. A **21**, 3815 (1988).