Extinction, Survival, and Dynamical Phase Transition of Branching Annihilating Random Walk

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We analyze statistical properties of random walkers which disappear when they meet and make offsprings by a controllable rate. Numerical results for one, two, and three dimensions and for the Sierpinski gasket are assessed in view of the mean-field theory predictions. Universality classes are found to depend on the number of offsprings in space dimension less than 3.

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In recent years diffusion-limited annihilation of the type $A+A\rightarrow 0$ has received a lot of attention (see [1,2] and references in them). With one of the most important real-life examples of identical particle annihilation being the free radical recombination in chemical chain reactions, it would be natural to add to this process a branching step $A\rightarrow(n+1)A$ in order to accommodate a vast category of branching chain reactions, covering many important oxidation processes [3]. Defining this process on a lattice leads us in the diffusion-controlled limit to a branching annihilating random walk, a process first introduced by Bramson and Gray [4].

The branching annihilating random walk (BAW) of particles occupying sites of a lattice is a process comprising two steps, taking place with probabilities p and $1-p$, respectively. (1) A particle is chosen at random and moves to a randomly chosen nearest-neighboring site. If this site is already occupied, the two particles annihilate leaving an empty site. (2) A particle, chosen at random, produces a fixed number of offsprings which are placed on neighboring sites. If a newborn offspring tries to occupy an already occupied site, it annihilates with the occupying particle leaving an empty site.

In the course of BAW, particles can eventually disappear (extinction) or a nonzero concentration of particles can exist indefinitely (survival). One can easily show that in even-offspring BAW, parity of the total number of particles is preserved. Further we assume that the initial number of particles is even, so that extinction is possible in principle.

It was shown rigorously by Bramson and Gray [4] that one-offspring BAW in one dimension survives at sufficiently small p, while if the value of p is big enough the particles are eventually eliminated. Sudbury [5] proved the extinction of two-offspring BAW in one dimension at any $p>0$.

The outline of the current article is as follows: First we present the mean-field results, derived for an arbitrary number of offsprings and any dimensionality; then we present the results of numerical simulations in one, two, and three dimensions and on the Sierpinski gasket; and finally we present an exact treatment of the particle extinction dynamics of two offsprings in one dimension.

In order to construct a mean-field theory for BAW on a lattice with coordination number z let us choose a site and consider its neighbors as mean-field sites. Now only events leading to a change in the state of the chosen site will be considered. When the chosen site is empty, which happens with probability $1-c$, where c is the concentration of particles, two events must be taken into account: (1) A particle jumps from a mean-field site to the chosen site, and (2) a mean-field-site particle puts an offspring on the chosen site. When the chosen site is occupied we must also consider jumping of a particle from the chosen site. By assuming that the particle concentration of the mean-field sites is equal to that of the chosen site, we obtain

$$\frac{d}{dt}c(t)=\frac{1}{z+1}[(1-c)\{cp+nc(1-p)\}-c\{cp+nc(1-p)+p\}]=\frac{1}{z+1}c\{(1-p)n-2c(n+p-np)\}, \tag{1}$$

where n denotes the number of offsprings. The fixed points of (1) are

$$c=0,\quad \frac{n(1-p)}{2(n+p-np)}. \tag{2}$$

It can be shown that the first solution is unstable. The stable solution is monotonically decreasing with p, giving $c=\frac{1}{2}$ at $p=0$ and $c=0$ at $p=1$. Namely, we have survival at any p except the case of no branching ($p=1$). Using terminology of phase-transition theory we may summarize the mean-field results as follows: A dynamical phase transition from survival to extinction occurs at the value of control parameter $p=1$ with the critical exponent for concentration $\beta=1$.

Numerical simulations were performed on a 10000-site lattice in one dimension, on a 100×100 square lattice in two dimensions, and on a $20\times20\times20$ simple cubic lattice in three dimensions (with periodic boundary conditions). In order to introduce multiple branching we had to make a convention on how to place the offsprings around the origin. We placed the offsprings in the most compact manner possible; that is, keeping the center of mass of the sites, receiving the offsprings, as close to the original particle as possible. In the cases where there were several equivalent most compact configurations, we used all these

TABLE I. Check of size dependence: calculated critical probabilities (p^*) and critical exponents (β) at different lattice sizes (two-dimension one-offspring case).

Size	p^*	β
25×25	0.96	1.5
50×50	0.85	1.0
80×80	0.85	1.0
100×100	0.85	1.0

configurations with equal probability.

We approximated the Sierpinski gasket by a 29526-site lattice, obtained by making nine iterations of the usual transformation, leading to the true Sierpinski gasket in the limit of infinite number of iterations. For the Sierpinski gasket we put the required number of offsprings completely at random on the sites, neighboring the original site. In the case of the Sierpinski gasket we used reflective boundary conditions; that is, each site had four nearest neighbors, except for the three sites in the corners, which had two nearest neighbors each.

We judged a BAW to survive if the number of steps per lattice site, starting from a lattice completely covered with particles, exceeded 10000 without reaching the extinction state with zero concentration of particles. Doubling this arbitrary number did not affect the steady-state concentrations of particles, except for the two-offspring BAW in one dimension, when what seemed to be a small survival region was rapidly shrinking with the increase of the maximal number of steps, which led us to the conclusion that there is no survival at any $p > 0$.

We calculated the steady-state particle concentration dependence on the value of p for a mesh of p values taken with a step 0.01, starting from $p = 1$. When the transition between survival and extinction was detected (that is, when a point with nonzero concentration of particles after 10000 steps per site of the lattice is reached), we fitted the data in the vicinity of the threshold as $c \sim (p - p^*)^\beta$ (usually taking seven points with a nonzero stationary concentration of particles) and considered the values of p^* and β which gave the best fit as the best approximation for the true values of the threshold jump probability and critical exponent.

To make sure that the same power-law dependence was holding up to the transition point we tried to use a 0.001 mesh to estimate p^* and β values. We were able to obtain values consistent with the results for the 0.01 mesh in all cases except four offsprings in one dimension and one offspring in two dimensions, where the data for the 0.001 mesh were too scattered at the system size we used to make any assessment of p^* and β.

In order to check the size dependence we changed the size of the lattice by a factor of 2 or 3. In all cases no significant or systematic change in the values of stationary concentrations has been detected. For the case of one offspring in two dimensions we have estimated p^* and β on the basis of data obtained for different lattice sizes. The results, indicated in Table I, clearly show that our approach to the estimation of p^* and β gives consistent results for a wide range of lattice sizes.

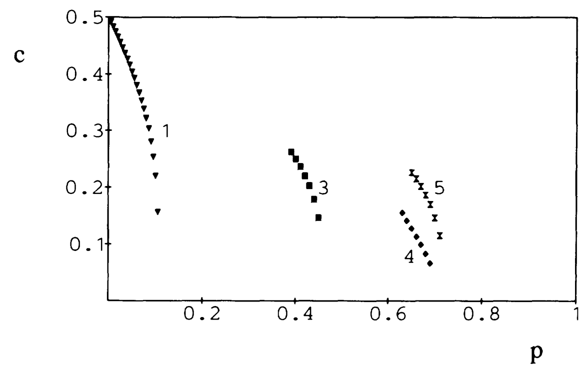

FIG. 1. One dimension: Steady-state concentrations of particles near the threshold. Numbers indicate the number of offsprings.

The results of our simulations are presented in Figs. 1 through 4 and in Table II. The mean-field prediction of survival at any $p < 1$ proved to be valid for any number of offsprings in the three-dimensional case. For two dimensions a nontrivial threshold value was obtained for the one-offspring BAW. In one dimension we found $p^* \neq 1$ at all numbers of offsprings considered.

For the one-offspring BAW in one dimension our results confirm the prediction of the existence of a nontrivial critical point made by Bramson and Gray [4] and for the two-offspring BAW, the prediction by Sudbury [5] of extinction at any $p > 0$. In one dimension, $p^* = 0$ in the two-offspring case and p^* is nontrivial in other cases. The cases of odd numbers of offsprings seem to belong to the same universality class while the case of four offsprings gives a different critical exponent.

In two dimensions a set of BAWs with the number of offsprings greater than 1 seems to form a universality class with $\beta \neq 1$, while the value of p^* is less than 1 in the

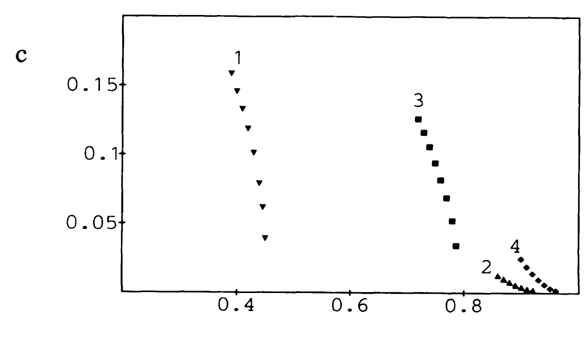

FIG. 2. Sierpinski gasket: Steady-state concentrations of particles near the threshold.

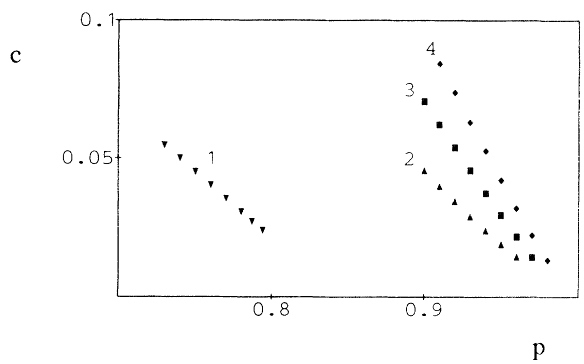

FIG. 3. Two dimensions: Steady-state concentrations of particles near the threshold.

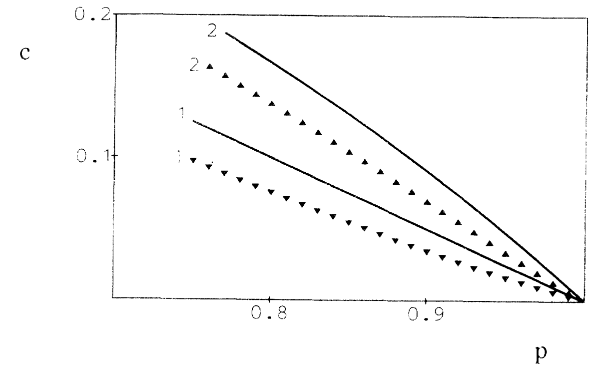

FIG. 4. Three dimensions: Steady-state concentrations of particles near the threshold. Mean-field theory predictions are shown by solid lines.

case of one offspring.

All three-dimensional BAWs have the mean-field values of $p^*=1$ and $\beta=1$. This result seems to indicate that the critical dimension is two. However, the actual values of stationary concentrations near the threshold do not follow Eq. (2); namely, the critical coefficients are different (see Fig. 4). Therefore, we know that the spatial restriction cannot be neglected even in three dimensions.

Our simulations of the Sierpinski gasket reveal a striking difference between the odd and even numbers of offspring cases, which seem to form two separate universality classes. On the Sierpinski gasket two- and four-offspring BAWs follow the mean-field theory prediction of $p^*=1$.

In order to check the mean-field theory prediction of $c=0.5$ at $p=0$, we performed simulations for all dimensionalities and offsprings numbers listed in Table II. In all cases this prediction has been confirmed by simulations (although it is possible to show exactly that in some special situations with the number of offsprings close to the size of the system this mean-field theory prediction is not valid [6]).

The most interesting point may be the dependence on parity. In the case of even offspring the parity of the particle number is conserved, and this conservation law may give rise to the even-odd differences in one dimension and on the Sierpinski gasket. In the case of odd offspring there is a possibility that a particle produces an odd number of particles and they all annihilate by random walks. Therefore, the odd offspring cases may be more likely to die than the even offspring cases. This intuitive estimation is valid for the Sierpinski gasket and for two dimensions with one offspring. The reason that the value of p^* for five offspring is less than that for four offspring in one dimension may also be explained by this effect.

An exception of this intuition is the case of two offspring in one dimension where we have only the extinction state for all nonzero p. This special case can be analyzed rigorously as follows [7]. Let $m_j(t)=1$ when there is a particle at time step t on the jth site, and $m_j(t)=0$ otherwise. Then $m_j(t+1)$ is given probabilistically as

$$m_j(t+1)=\begin{cases} m_j(t), & \text{probability } 1-2/N, \\ 0, & \text{probability } p/N, \\ m_j(t)+m_{j-1}(t) \bmod 2, & \text{probability } (1-p)/N+p/2N, \\ m_j(t)+m_{j+1}(t) \bmod 2, & \text{probability } (1-p)/N+p/2N, \end{cases} \quad (3)$$

TABLE II. Critical probabilities (p^*) and critical exponents (β).

Number of offspring	1D p^*	1D β	Sierpinski gasket p^*	Sierpinski gasket β	2D p^*	2D β	3D p^*	3D β
1	0.108 ± 0.001	0.32 ± 0.01	0.45 ± 0.01	0.5 ± 0.1	0.85 ± 0.01	1.0 ± 0.1	1.00 ± 0.01	1.0 ± 0.1
2	0	...	1.00 ± 0.01	3.0 ± 0.3	1.00 ± 0.01	1.25 ± 0.02	1.00 ± 0.01	1.0 ± 0.1
3	0.461 ± 0.002	0.33 ± 0.01	0.79 ± 0.01	0.5 ± 0.1	1.00 ± 0.01	1.26 ± 0.02	...	...
4	0.72 ± 0.01	0.7 ± 0.1	1.00 ± 0.01	3.0 ± 0.3	1.00 ± 0.01	1.25 ± 0.02	...	...
5	0.718 ± 0.001	0.33 ± 0.01	...	...	...	...	...	...

where N denotes the system size and the pair-annihilation effect is represented by taking mod2. Let us consider the probability Q_r that the number of particles on r consecutive sites is odd. First let us note that Q_1 is equal to the concentration of particles c and that $Q_N=0$ (N is the total number of sites) because the total number of particles is always even. From Eq. (3) we have the following equation for Q_1:

$$Q_1(t+1)=Q_1(t)+\frac{1}{N}[-2Q_1(t)+(2-p)Q_2(t)]\,. \qquad (4)$$

By considering the stochastic time evolution of the sum of r consecutive sites as we did for $m_j(t)$, we can get equations for Q_r for $r=2,3,\ldots,$ as

$$Q_r(t+1)=Q_r(t)+\frac{2-p}{N}[Q_{r-1}(t)-2Q_r(t)+Q_{r+1}(t)]\,. \qquad (5)$$

This set of equations makes a discretized diffusion equation in (r-t) space and it can be shown that the only steady-state solution for $p\neq 0$ is $Q_1=Q_2=\cdots=0$, which means extinction. In the case of no random walk ($p=0$) a survival solution ($Q_1=Q_2=\cdots\neq 0$) is possible.

As Eq. (5) is an ordinary diffusion equation we can estimate that $c(t)$ decays following $1/\sqrt{t}$ for large t in the limit of $N\to\infty$. This estimation is not rigorous because Eq. (4) for $r=1$ is a little modified from the ordinary diffusion equation, but it is confirmed numerically that such decay really takes place for large enough t (typically $t\gg 1000$) whenever $p\neq 0$.

In summary, by varying the number of offsprings and dimensionality of the underlying lattice we have found a variety of steady-state behaviors in the system of branching annihilating random walkers. For one dimension with more than three offsprings and for the Sierpinski gasket, we have no rigorous theory yet, but parity conservation seems to be playing a central role in the universality classes.

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[6] For example, in the case where the system size N is equal to $n+1$ the number of particles oscillates deterministically as k, $N-k+1$, k, $N-k+1,\ldots,$ where k denotes the initial number of particles, which leads to $c=(N+1)/2N\neq 0.5$.
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