$A + A \rightarrow \emptyset$ model with a bias towards nearest neighbor

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We have studied the $A + A \rightarrow \emptyset$ reaction-diffusion model on a ring, with a bias ϵ ($0 \leqslant \epsilon \leqslant 0.5$) of the random walkers A to hop towards their nearest neighbor. Though the bias is local in space and time, we show that it alters the universality class of the problem. The z exponent, which describes the growth of average spacings between the walkers with time, changes from the value 2 at $\epsilon = 0$ to the mean-field value of unity for any nonzero ϵ. We study the problem analytically using independent interval approximation and compare the scaling results with those obtained from simulation. The distribution $P(k,t)$ (per site) of the spacing between two walkers is given by $t^{-2/z} f(k/t^{1/z})$ and is obtained both analytically and numerically. We also obtain the result that ϵt becomes the new time scale for $\epsilon \neq 0$.

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I. INTRODUCTION

Diffusion-controlled annihilation problems have received lots of attention over the years [1–16]. These are nonequilibrium systems of diffusing particles, which undergo reactions such as pairwise annihilation. Depending on the problem, these particles may represent molecules, biological entities, opinions in societies, or market commodities and such systems are widely used to describe the pattern-formation phenomena in wide varieties of biological, chemical, and physical systems. In the lattice version of the simple single species problem, each lattice site is filled with a particle at time $t = 0$. At each time step, the particles are allowed to jump to a nearest neighbor site. In general no preferred direction for the jump is assigned. Particles react only when a certain number k of them meet: $kA \rightarrow lA$ with $l < k$. Annihilating random walkers with $k = 2$ and $l = 0$ mimics the dynamics of voter models and the Glauber-Ising model in one dimension. Such systems have been studied in one dimension [6–13] as well as in higher dimensions [17–20]. The steady state of the process is rather simple. Depending on the initial condition, whether one starts with an even or an odd number of particles, the steady state will contain no particles or one particle, respectively. The focus in all these analyses is how the system approaches the steady state. In particular, one wants to know how the number of particles decay with time and how the distribution of the intervals between the particles evolves with time.

The dynamics of the system is governed by two processes: reaction (annihilation) and diffusion. If the reaction time much exceeds the diffusion time, the process is reaction limited. In this regime, the kinematics is dominated by the diffusion and it is well described by the mean-field equations. On the other hand, in the diffusion-limited regime, where the diffusion time is much larger than the reaction time, the process is dominated by the fluctuations caused by the reaction and, at low dimensions, kinetics is no longer described by mean-field rate equations. For the $A + A \rightarrow \emptyset$ model ($k = 2$ and $l = 0$), the critical dimension d_c is 2. For dimension $d > d_c$, the mean-field behavior is valid, which indicates that the density of the particles decays with time as $1/t$ for a random initial configuration of the particles. In the mean-field picture, the time scale is set by the reaction rate, which at high dimensions is given by the average steady-state flux of the particles towards any particle in the system.

At low dimensions, for $d \leqslant 2$, the problem of the recurrence of random walks appears. From the point of diffusion, the collision rate is effectively infinite. The rate equation gives the asymptotic behavior of the density of particles $N_p(t)$ decaying as $\sim 1/t^{1/z}$ for $d < d_c$, with $z = 2$. The average domain size or interval (i.e., the distance between neighboring walkers in one dimension) D_s scales as $t^{1/z}$ and this is the only length scale which characterizes the reactant distribution. The scaling is robust as long as the particle motions are uncorrelated and diffusive with well-defined mean and fluctuation. At $d = d_c$, the mean-field result is retrieved with logarithmic corrections. The value of d_c and the behavior of $N_p(t)$ have been conjectured by scaling arguments [17], exact results in one dimension [7,8,12,21], probabilistic approaches [5,6], and renormalization group calculations [18,20,22,23].

Here, we present the study of the time evolution of a set of randomly distributed random walkers on a ring, having the interaction $A + A \rightarrow \emptyset$, evolving with the following dynamical rule: at each time step each walker moves towards its nearer neighbor with a probability $1/2 + \epsilon$. $\epsilon = 0$ would give the usual unbiased random walkers while for $\epsilon = 1/2$ the walkers will always move towards their nearer neighbors, making the system quasideterministic. When the two neighbors are at the same distance the particle moves either way with equal probability. The ring geometry is taken to impose the periodic boundary condition. We call this model the anisotropic walker model (AWM) hereafter. The AWM is motivated by the social phenomenon of opinion formation and, for $\epsilon = 1/2$, coincides with the binary opinion dynamics/spin model (BS model) proposed in Ref. [24].

The BS model was proposed to mimic opinion formation in a society where the opinions are binary. Here an agent's opinion is decided by the size of the neighboring domains (in a domain all opinions are of the same type) which may be interpreted as social pressure. In the BS model, surprisingly, it was found that $z \simeq 1$. That means ϵ alters the universality class

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of the problem. The generalization of the model with $\epsilon > 0$ implies that an agent in the BS model follows the opinion of the larger domain with a probability (larger than 0.5) which makes the system fully stochastic.

Simulations of the AWM with rather small sizes indicated [25] that any ϵ in the range $0 < \epsilon \leqslant 1/2$ alters the value of the exponent z compared to the case $\epsilon = 0$ [26]. Here, we study the AWM to understand the effect of ϵ on the long time behavior of the $A + A \to \emptyset$ model. We study, particularly, the distribution $P(k,t)$ of the interval sizes (the distance between the neighboring walkers equivalent to the domains in the opinion formation model) k per site at time t and its evolution with time. This distribution is of importance as it helps analyzing the dynamic process and has been calculated in many dynamical models in one dimension. Often the mapping with Glauber spin picture is utilized to evaluate this function. The present model, however, is not equivalent to a Glauber-like model and thus one may expect the results to be different in general.

We obtain the scaling solution of $P(k,t)$ for late times; it is of interest to check whether nonzero values of ϵ can alter the known form for $\epsilon = 0$. We have employed the independent interval approximation (IIA) (described below) to study the evolution analytically and have complemented the findings with Monte Carlo simulation results.

II. IIA ANALYSIS

The IIA was originally proposed in Ref. [27] and has been applied to several studies of the diffusion-limited processes. The IIA implies that the intervals or gaps between the nearest neighboring particles are independent of each other. The IIA has been successfully applied to the case of diffusion-limited annihilation $A + A \to \emptyset$ (which maps to the Glauber spin model) to obtain the interparticle interval distribution function [28]. In simple diffusion problems, the idea of the IIA has been used to predict the persistence exponents in excellent agreement with the simulation results [29,30].

The assumption that the intervals or domains are uncorrelated was later developed self-consistently for several models in Ref. [31]. In particular, the IIA analysis describes the dynamics of the model for $\epsilon = 0$ extremely well [28,31,32], qualitatively. The quantitative accuracy increases if one uses the exact expression of the equal-time two-spin correlation function along with the IIA [28]. We show here that the analysis can be extended to the nonzero ϵ case also. The IIA analysis gives the scaling form for $P(k,t)$ with the scaling exponent $z = 1$ and also gives the exponential decaying form of the scaling function. The IIA results are well supported by numerical simulation results. Our results show that ϵt becomes the new time scale for nonzero ϵ. As a result, at low ϵ, it takes a longer time to reach the asymptotic scaling limit.

Within the IIA, the master equation that describes the rate of change of $P(k,t)$ (written $P(k)$ for brevity) with time can be broken into ϵ-independent and ϵ-dependent terms and is given by

$$\frac{dP(k)}{dt} = I_1(k) + 2\epsilon I_2(k), \tag{1}$$

where

$$I_1(k) = P(k+1) + P(k-1) - 2P(k) + \frac{P(1)}{N^2} \times \left[\sum_{m=1}^{k-2} P(m)P(k-m-1) - N[(P(k) + P(k-1)]\right] \tag{2}$$

and

$$\begin{aligned} I_2(k) = {} & \frac{P(k+1)}{N}\left[\sum_{m>k+1} P(m) - \sum_{m<k+1} P(m)\right] \\ & + \frac{P(k-1)}{N}\left[\sum_{m<k-1} P(m) - \sum_{m>k-1} P(m) - P(1)\right] \\ & \times (1 - \delta_{k,2}) - \frac{P(k)P(1)}{N^2}\sum_{m>1} P(m) + \frac{P(1)}{N^2} \\ & \times \left[\sum_{m>1}^{k-2} P(m)P(k-m-1) - P(1)P(k-m-1)\right] \\ & - P(1)\left[1 - \frac{P(1)}{N}\right]\delta_{k,2}, \end{aligned} \tag{3}$$

where $N = \sum_k P(k,t)$ is the density of the intervals (number of intervals per lattice site) at time t and is equal to the density of the particles A at time t. Naturally, $\sum_k kP(k) = 1$, which comes from the conservation of the total length of all the intervals. The details of the derivation of Eq. (1) are given in the Appendix.

The $\epsilon = 0$ case, which corresponds to $I_1(k)$ in Eq. (1), has been studied before using the IIA [31]. $P(k,t)$ is found to have the expected scaling form:

$$P(k,t) = t^{-2/z} f\left(\frac{k}{t^{1/z}}\right), \tag{4}$$

with the scaling exponent $z = 2$. The scaling function $f(x) \sim \exp(-\alpha x)$ at large x. The average length k of the intervals at time t: $\langle k(t)\rangle = \int kI_1(k)dk / \int I_1(k)dk \propto t^{1/z}$. The scaling behavior given by Eq. (4) matches that obtained from the exact analysis of the model [32] except for the value of α. It should be noted that $\sum_k I_1(k) = N$, $\sum_k kI_1(k) = 1$ (normalization condition), and $\sum_k \frac{dI_1(k,t)}{dt} = \frac{dN}{dt} = -2P(1)$. The last result implies that any change in N is brought out by the annihilation of two A particles which were at a unit distance apart and coalescence of the intervals separated by these two particles.

For nonzero ϵ, the term $I_2(k)$ appears in the rate equation. It should be noted that $\sum_k I_2(k) = 0$, $\sum_k kI_2(k) = 0$ and $\sum_k \frac{dI_2(k)}{dt} = -\epsilon P(1)[1 + \frac{P(1)}{N}]$. We solve Eq. (1) numerically starting with intervals of sizes $1,2,\ldots,n$ with distribution $P(k,0) = \eta_1\delta_{k,1} + \eta_2\delta_{k,2} + \cdots + \eta_n\delta_{k,n}$, where $\eta_1,\eta_2,\ldots,\eta_n$ are random numbers between 0 and 1 and $\eta_1 + 2\eta_2 + \cdots + n\eta_n = 1$. We find that the final result is insensitive to the choices of η's or the number of different types of intervals to start with or different configurations of the starting interval distribution. Most of our analytical results are obtained with initial intervals of size $n \leqslant 3$ and averaged typically over ten

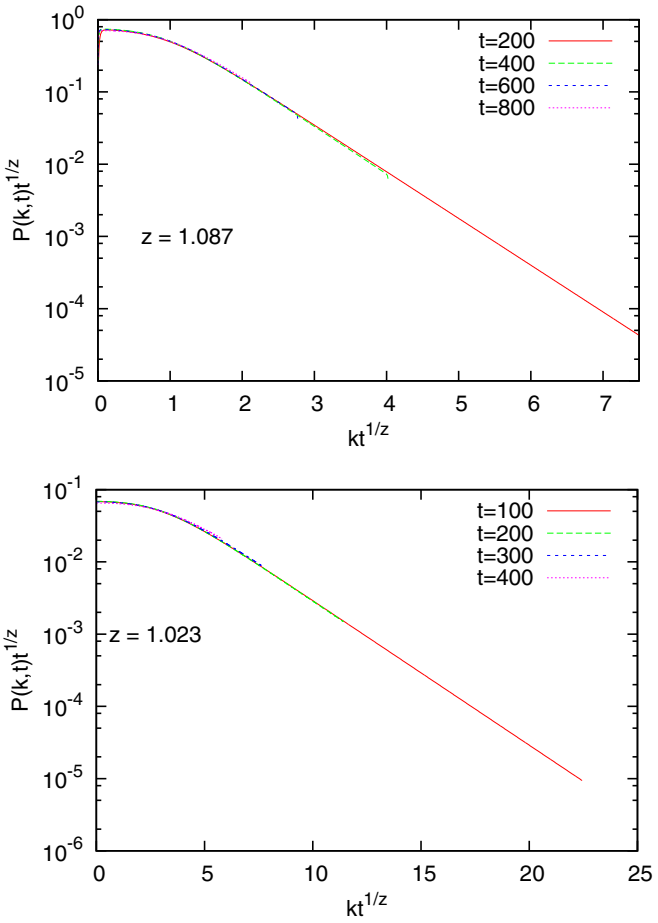

FIG. 1. (Color online) The scalings of the interval size distributions $P(k,t)$ obtained from the IIA for $\epsilon = 0.1$ and 0.5 are shown at different times t.

different initial configurations. On the other hand, we find that the results depend crucially on the discrete time step involved in Euler's method and the observation time. In most of our results, time is incremented by $\delta t = 0.01$ at each step. We have studied systems of sizes $L = 1000$ and 2000. We find that this gives us a good idea of the validity of the scaling and the exponential decay of the scaling function at large arguments at the expense of a reasonable computer time. It may also be added that the value of L enters the numerical calculation indirectly as the rate equation is in terms of probabilities and L determines only the upper bound of the size of the domains. We check that z approaches the values 2 and 1 at $\epsilon = 0$ and 0.5, respectively, as δt is lowered for $L = 2000$ and there is no appreciable finite size effect.

For nonzero ϵ, the solution of Eq. (1) obtained numerically shows that $P(k,t)$ retains the same scaling form as in Eq. (4). One can obtain a collapse by suitably scaling the variables using trial values of z for each ϵ. Figure 1 shows the scaling for two specific values of ϵ at four different times. The dependence of z on ϵ is shown in Fig. 2. For $\epsilon < 0.1$, z shows a relatively sharp increase to $\sim$2.0 as $\epsilon \to 0.0$. However, above $\epsilon = 0.1$, the variation is not systematic, which suggests that the value is actually a constant. The values of z in this region differ from 1 by not more than 10%. The data collapse using using Eq. (4)

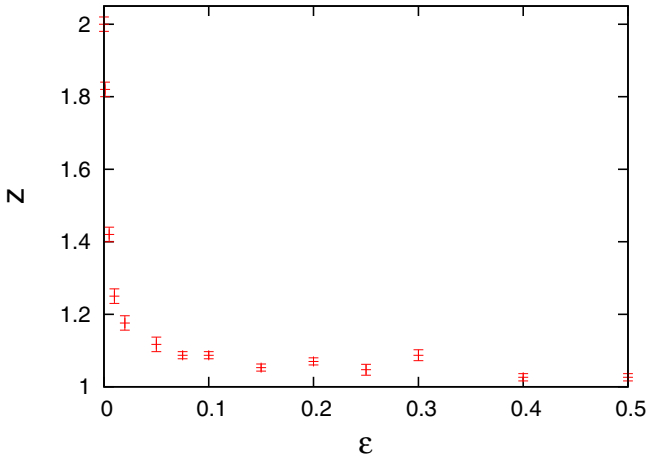

FIG. 2. (Color online) Values of z (along with error bars) obtained using the IIA are plotted against ϵ.

which we have used to extract the value of z is insensitive to this small fluctuation in the value. In principle, one can think of a functional dependence of z on ϵ but other results (such as the scaling behavior in Eq. (5) appearing later in the paper) indicate that the variation of z for $\epsilon > 0$ is only an artifact of the sudden change in z at $\epsilon = 0$ and actually z is a constant in this region. This is supported by the fact that the sharp rise of z occurs at lower ϵ values as one increases the observation time (in the scaling regime). We thus conclude that the IIA method gives $z = 1$ for all $\epsilon \neq 0$ and 2 only when $\epsilon = 0$, consistent with earlier results obtained from simulations in Ref. [25]. We also show below that, for $\epsilon > 0$, the cumulative distribution gives consistent results with that obtained theoretically, using $z = 1$, to support our conclusion.

Using the form of $P(k,t)$ given by Eq. (4), one can calculate the cumulative distribution $Q(k,t) = \sum_{m=1}^{k} m P(m,t)$. Assuming an exponential behavior of the scaling function [$f(x) \sim \exp(-\alpha x)$], one gets $Q(k,t) = 1 - \exp(-\alpha k/t^{1/z})(1 + \alpha k/t^{1/z})$. In Fig. 3 we plot the cumulative

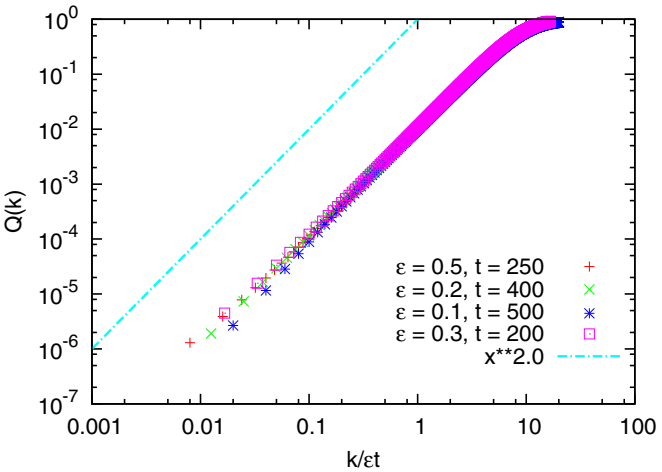

FIG. 3. (Color online) The cumulative distribution $Q(k,t) = \int_0^k n P(n) dn$ from the IIA for nonzero ϵ. The straight line has slope = 2.0.

distribution $Q(k,t)$ as obtained from IIA calculations for different values of ϵ and times t. The distribution exhibits the scaling $Q(k,t) \sim h(\frac{k}{t})$, which is consistent with the value $z = 1$. The scaling function appearing in the cumulative distribution behaves like $h(x) \sim x^{\delta}$ for small x and goes to unity at large x. The value of δ is close to 2, which agrees with the theoretical estimate when $k/t^{1/z}$ is small. We note another interesting feature; the curves for different values of ϵ collapse when the data are plotted against $k/(\epsilon t)$, such that the behavior of $Q(k,t)$ may be written as

$$Q(k,t) \sim h\left(\frac{k}{\epsilon t}\right). \tag{5}$$

We get back to this behavior later in Sec. IV.

III. SIMULATION RESULTS

We verify the scaling results by Monte Carlo simulation. We start (at $t = 0$) with a one-dimensional chain of size L with half of the lattice sites occupied randomly by the particles A. L is varied between 10^4 and 10^5 and the periodic boundary condition is used. In a single update, we choose a site randomly and if there is a particle its position is updated. L such updates constitute one Monte Carlo step and the dynamics is asynchronous. The distances (in terms of lattice units) of the neighboring particles are obtained and the particle is shifted one lattice site left or right with probability $(1/2 + \epsilon)$ towards the nearer neighbor and $(1/2 - \epsilon)$ along the other direction. If the new site is occupied, then both the particles occupying that site and the one which has hopped over to it are removed from the system. As ϵ is made larger, the rate of annihilation becomes high and as a result very few walkers remain at large times. This poses a difficulty in obtaining good statistics of the data for the distribution $P(k,t)$. One has to carefully identify the scaling regime which is almost nonexistent for small systems. Hence, for this analysis, $L = 5 \times 10^5$ was used for which the scaling regime can be obtained only for small values of time t. For small ϵ values, a system size of $L = 10\,000$ suffices. The data are averaged typically over 1000 different random initial configurations of the positions of the particles. For $\epsilon = 0$, $P(k,t)$ follows Eq. (4) as in the IIA with $z = 2.0$.

Before discussing $P(k,t)$ for nonzero ϵ, we check that for the large system sizes considered, the fraction of surviving walkers shows the scaling $N_p \propto t^{-1}$ (see Fig. 4) and there is no need to consider any correction to scaling (for any value of ϵ) reported earlier [25] for comparatively smaller sizes. The results for $P(k,t)$ are plotted in Fig. 5. We report results for $\epsilon \geqslant 0.1$ which show agreement with the scaling behavior as given in Eq. (4) (shown in Fig. 5). The value of z shows deviation from unity only for the smallest value of ϵ. We also estimate the cumulative function $Q(k,t)$ which again shows a collapse when plotted against $x = k/\epsilon t$ for $x > 1$ (see Fig. 6). However, although $Q(x) \propto x^{\delta}$ as obtained in the IIA, the exponent δ has a lower value of $\sim$1.8. We also make a further analysis: if Eq. (5) is obeyed with $h(x) \propto x^{\delta}$, $\log[Q(x))/Q(x/b)]$ must be equal to $\delta \log b$ where b is a scaling factor. Estimating δ in this way, we find $\delta \approx 1.78$ (see the inset of Fig. 6). This plot has been done for small values of x where the power-law behavior is expected to be valid; for large values of the argument, $Q(x)$ approaches unity as it is a cumulative probability.

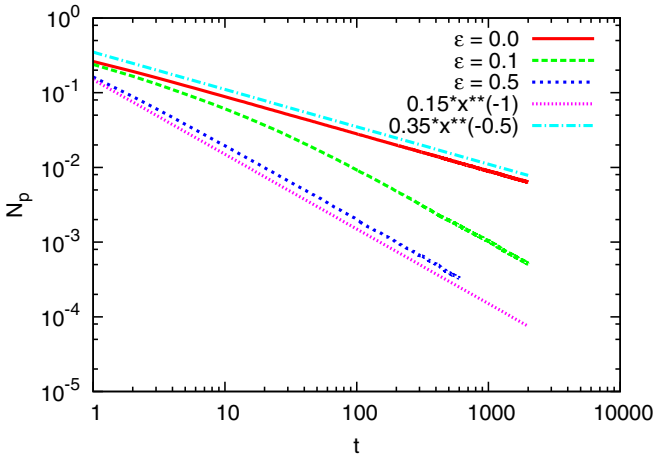

FIG. 4. (Color online) N_p versus t from simulations for different values of ϵ.

IV. DISCUSSIONS AND CONCLUDING REMARKS

In this paper, we have used two approaches to study the AWM. The results of the IIA approach and the simulations agree quite well but the values of α (associated with the scaling function f) differ notably (e.g., α for $\epsilon = 0.5$ is approximately 0.45 from the IIA while simulations give a value of $\sim$0.26). This, however, is not surprising as, even for $\epsilon = 0$, $\alpha \approx 0.55$ [31] is quite different from the exact result (0.368 468) [32].

Another difference which appears is the disagreement of the value of δ (associated with the scaling function h) in the two methods. The theoretical value $\delta = 2$ is derived assuming the scaling function f occurring in Eq. (4) has an exponential decay which is true for large values of the argument of f in both cases. The discrepancy in the value of δ thus suggests that for small values of the argument there may be a significant difference in the form of the scaling function in the IIA and the simulation results. However, this region where the difference is speculated to occur is rather narrow to make a systematic study.

The result that $k/\epsilon t$ appears as the scaling variable, obtained in both the approaches, immediately suggests that α in Eq. (4) varies as $1/\epsilon$. We note the values of $\alpha\epsilon$ to check whether this is true and find good agreement for the IIA values for $\epsilon \geqslant 0.3$ and very good agreement for the values obtained in simulation for $\epsilon > 0.1$. $\alpha\epsilon \sim 0.13$ for $\epsilon > 0.1$ (from the simulation results), while it apparently decreases for lower values of ϵ. However, as we have noted earlier, the results for very small ϵ show the effect of the $\epsilon = 0$ point which belongs to a different universality class. Since the α value obtained from the simulation happens to be more reliable, we conclude that indeed $\alpha \propto 1/\epsilon$ for all values of $\epsilon > 0$.

To summarize, we have considered the $A + A \to \emptyset$ reaction-diffusion model on a ring, with a bias ϵ $(0 \leqslant \epsilon \leqslant 0.5)$ of the random walkers A to hop towards their nearest neighbor. The interval size distribution $P(k,t)$ is evaluated using the

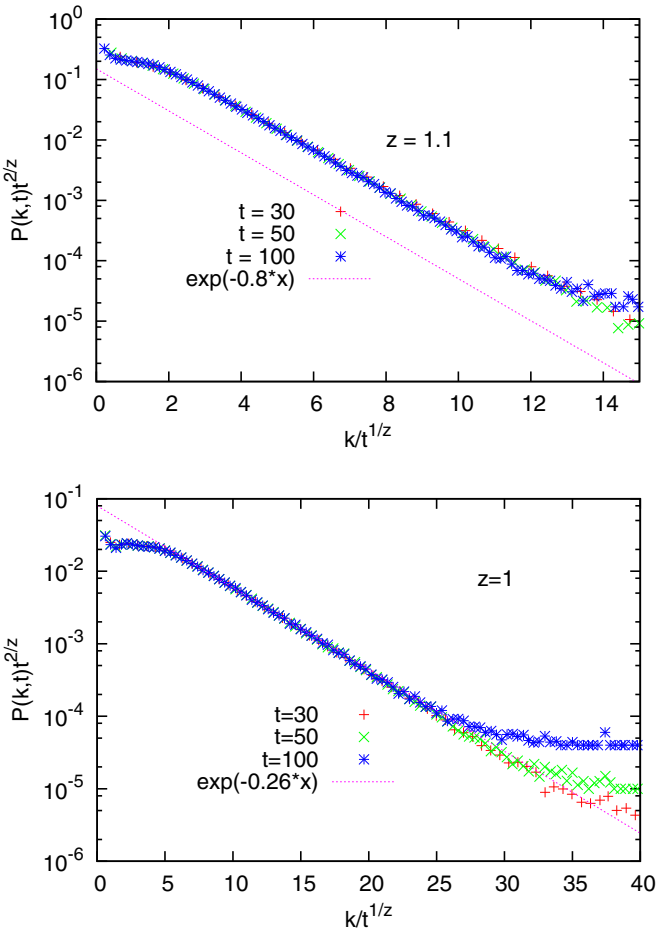

FIG. 5. (Color online) The scalings of the interval size distributions $P(k,t)$ from simulation for $\epsilon = 0.1$ and 0.5 at times $t = 30$, 50, and 100 are shown. The scaling holds good for $1/z = 0.91$ and $1/z = 1.0$, respectively.

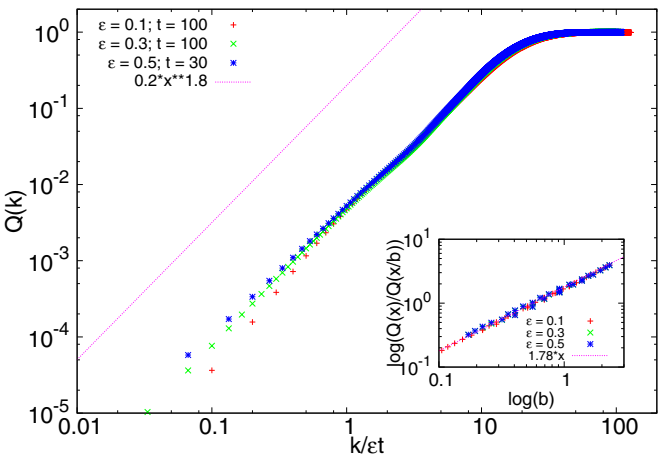

FIG. 6. (Color online) The cumulative distribution $Q(k) = \int_0^k nP(n)dn$ for $\epsilon = 0.10$; $t = 100$, $\epsilon = 0.30$; $t = 100$, and $\epsilon = 0.5$; $t = 30$ is plotted against $k/\epsilon t$. The straight line has slope = 1.8. The inset shows the log-log plot of the ratio of two values of Q at x and x/b against b where b is a scaling factor.

IIA method and compared to results obtained from numerical simulations. Both the methods show that for $\epsilon \neq 0$, the exponent $z = 1$ in contrast to $z = 2$ for $\epsilon = 0.0$. The raw data may not give the value of z for $\epsilon \neq 0$ very accurately in the IIA, but the cumulative distribution function $Q(k,t)$ shows that the scaling variable is indeed k/t for $\epsilon \neq 0$. The exponential form of the scaling function $f \sim \exp(-\alpha x)$ for all ϵ values is also obtained by the IIA calculation and in simulation. The value of α however does not match between the IIA calculation and simulation for any ϵ. Simulation shows that $\alpha \sim 1/\epsilon$ for $\epsilon > 0.1$. We guess that this is true for all ϵ. Finally, we note that ϵt enters the scaling argument, implying a $1/\epsilon$ dependence of the time scale in the system.

As is mentioned in the Introduction, the diffusion and pairwise annihilation model has been studied a lot in the past in the context of modeling chemical reactions [33]. Systems of reacting particles are typical of complex irreversible nonequilibrium systems. It is crucial to ask what determines the universality class of the diffusing-annihilating particle system which is probably the simplest interacting particle system. Our study directly focuses on that. We show that our AWM yet again gives rise to a critical dynamics as the system approaches the steady state. We show that the exponent describing the dynamics changes from the value 2 to 1 as soon as the bias ϵ is introduced.

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APPENDIX: DERIVATION OF EQ. (1)

We consider the probability $P(k,t + \Delta t)$. It has contributions from several phenomena. Whenever we consider the movement of a domain wall, we have to compare the sizes of the two domains neighboring it. If the sizes are equal, the probability of a move to either side is simply 1/2.

The probability that a domain remains the same in size is $(1 - 2\Delta t)P(k)$. A domain of size $k + 1$ may reduce to a domain of size k if either of its two edges moves so as to shrink its size by 1. This probability will depend on the size of the adjacent domain, say m. If $m > k + 1$ such a move will happen with probability $(1/2 + \epsilon)$ and with probability $(1/2 - \epsilon)$ otherwise.

A domain of size $k - 1$ can also grow to a domain of size k. Once again, one has to take care of the size of the adjacent domain, m. It is convenient to consider the two cases $k > 2$ and $k = 2$ separately here. $k = 1$ will obviously not have any contribution from this process. For $k > 2$, moves will depend on whether $1 < m < k - 1$, in which case the probability is $(1/2 + \epsilon)$ while for $m > k - 1$ the probability is $(1/2 - \epsilon)$. One has to ensure that $m > 1$ in the first case, because for $m = 1$ a domain annihilation will take place. For $k = 2$, one has a domain of length unity growing to a domain of length 2 and this will be possible only for $m \neq 1$ and with probability $(1/2 - \epsilon)$.

A loss term will occur for the case when an adjacent domain of size 1 gets annihilated and this occurs with probability $(1/2+\epsilon)$ when another domain of size $m>1$ is its neighbor. If $m=1$, this occurs with probability 1/2. A gain term will also be there when two domains get annihilated and a domain of size k results in the process. Using the shortened notation $\epsilon_+ = 1+2\epsilon$, $\epsilon_- = 1-2\epsilon$, $k_+ = k+1$, and $k_- = k-1$, and taking care of all these terms, one gets

$$
\begin{aligned}
P(k,t+\Delta t) = (1-2\Delta t)P(k) &+ \Delta t \frac{P(k+1,t)}{\sum_k P(k,t)}\left[\epsilon_+ \sum_{m>k_+} P(m) + \epsilon_- \sum_{m<k_+} P(m) + P(k_+)\right] \\
&+ \Delta t \frac{P(k_-)}{\sum_k P(k)}\left[\epsilon_+ \sum_{1<m<k_-} P(m) + \epsilon_- \sum_{m>k_-} P(m) + P(k_-)\right](1-\delta_{k,2}) \\
&+ \Delta t\, P(1)\left[1 - P(1)/\sum_k P(k)\right]\epsilon_- \delta_{k,2} - \Delta t \frac{P(k)P(1)}{\left[\sum_k P(k)\right]^2}\left[\epsilon_+ \sum_{m>1} P(m) + P(1)\right] \\
&+ \Delta t \frac{P(1)}{\left[\sum_k P(k)\right]^2}\left[P(1)P(k-2) + \epsilon_+ \sum_{m>1}^{k-2} P(m)P(k_- - m)\right].
\end{aligned}
\tag{A1}
$$

For $\epsilon = 0$, the second and third terms can be rewritten as a single term and without using the Kronecker δ's.

[1] See, e.g, V. Privman, Editor, *Nonequlibrium Statistical Mechanics in One Dimension* (Cambridge University Press, Cambridge, UK, 1997); T. M. Ligget, *Interacting Particle Systems* (Springer-Verlag, New York, 1985); P. L. Krapivsky, S. Redner, and E. Ben-Naim, *A Kinetic View of Statistical Physics* (Cambridge University Press, Cambridge, UK, 2009), and the references therein.

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