

Random deposition of two annihilating species in the (1+1) dimension

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We present simulation results for the one-dimensional random deposition of two annihilating species A and B , falling with probabilities p and q ($p+q=1$), which then react to produce an inert product, i.e., $A+B\rightarrow 0$. Two different annihilation rules are defined: top annihilation and nearest-neighbor annihilation (NNA), leading to distinct scaling behaviors. In particular, the values of the scaling exponents for NNA are found to be dependent on probability p , suggesting different universality classes. [S1063-651X(99)01807-3]

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The formation, growth, and geometry of rough interfaces is a subject of great interest that has been extensively reviewed [1–5]. These studies play an important role in many phenomena of scientific interest and are relevant in a great variety of experimental situations, including the propagation of flame fronts, fluid flow in porous media, corrosion, material fractures, atomic deposition processes, and growth of bacterial colonies. Despite the diversity of these systems they have much in common, and it is possible to categorize them into universality classes. There are two main approaches for the theoretical analysis of such systems, one is based on computer simulations of discrete models, and the other describes the evolution of the interfaces by stochastic differential equations. The simplest discrete model for interface growth is random deposition (RD). Its simplicity is such that it allows us to determine the scaling exponents exactly, and to formulate a stochastic differential equation leading to the same scaling exponents [3].

The aim of the present paper is to simulate the random deposition of two annihilating species A and B (“particles” and “antiparticles”). The recombination of particles that collide during diffusion and react to form an inert product, i.e., the well-known reaction $A+B\rightarrow 0$, where 0 represents the inert product, is a simple example of nonequilibrium systems that have attracted a lot of interest [6–12]. This reaction leads to the segregation of like particles, and provides a useful model to also represent different physical systems such as the decay of lattice excitations, the monopole annihilation and surface reactions on supported catalyst.

It is quite simple to define the random deposition of two annihilating particles. First, a particle A or B , with probability p or q , respectively ($p+q=1$), is chosen to fall from a randomly located position over the surface. The selected particle follows a straight vertical trajectory until it reaches the surface, whereupon it sticks or reacts. If the falling particle is deposited on top of a column of its own kind or on a vacant column, the height of such a column is increased by 1. For the annihilating process, we can define two different rules, as in Fig. 1.

(i) Top annihilation (TA), a particle reacts only with antiparticles located at the top of a column.

(ii) Nearest-neighbor annihilation (NNA), a deposited particle on the top of a column reacts at random with any of its nearest-neighbor antiparticles, with the same probability.

In both situations the height of the reacting column decreases by 1, generating a single-valued interface, i.e., no overhangs are allowed. The former model is simpler and is introduced for comparison with the latter, which is more realistic from a physical point of view and leads to segregation of like particles. As is commonly defined, the unit time corresponds to the deposition of L particles on the interface, i.e., $t=N/L$ where N is the number of deposited particles and L is the number of columns or system size.

The profile of the evolving surface will gradually roughen under the stochastic deposition and annihilation of particles. Early simulations by Family and Viseck [13] suggested that in deposition processes of like particles, the surface roughness shows a dynamical scaling behavior.

To describe the discrete growth of an interface, it is useful to introduce two quantities [3]. The mean height of the surface $\langle h(t) \rangle$, is defined as

$$\langle h(t) \rangle = \frac{1}{L} \sum_{i=1}^L h(i,t), \quad (1)$$

where $h(i,t)$ is the height of column i at time t . For deposition processes with constant rate, the mean height increases linearly with time:

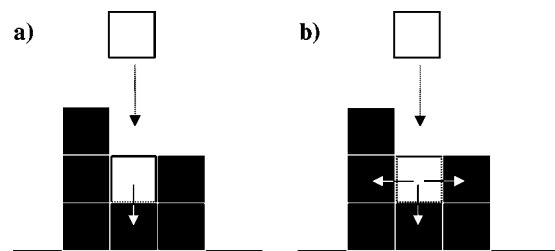


FIG. 1. In top annihilation (a), the B particle (empty square) reacts only with the A antiparticle (filled squares) below it. In nearest-neighbor annihilation (b), the B particle (empty square) reacts randomly with any of its nearest-neighbor A antiparticles (filled squares), with the same probability.

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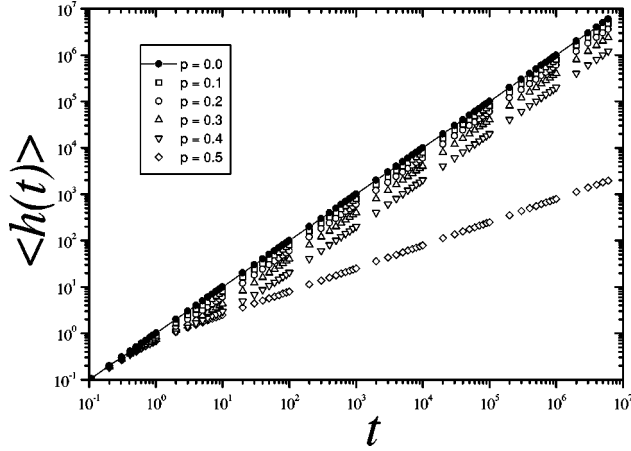


FIG. 2. Log-log plot for the time evolution of the average interface height $\langle h(t) \rangle$ with the TA rule, for different values of the probability p and fixed system size $L=75$. The asymptotic slopes are 1 for $p \neq 1/2$ and $1/2$ for $p = 1/2$. The unit time corresponds to the deposition of L particles on the interface, i.e., $t = N/L$ where N is the number of deposited particles and L is the number of columns or system size.

$$\langle h(t) \rangle \sim t. \quad (2)$$

The interface width $w(L, t)$, defined by the r.m.s. fluctuation in the height

$$w(L, T) = \left[\frac{1}{L} \sum_{i=1}^L [h(i, t) - \langle h(t) \rangle]^2 \right]^{1/2} \quad (3)$$

that characterizes the roughness of the interface.

Two different regimes, separated by a crossover time t^* can be distinguished.

(i) Growth regime, in which the width increases as a power of time,

$$w(L, t) \sim t^\beta \quad \text{for } t \ll t^*. \quad (4)$$

(ii) Saturation regime, during which the width reaches a saturation value that increases as a power of the system size L ,

$$w_{\text{sat}}(L) \sim L^\alpha \quad \text{for } t \gg t^*, \quad (5)$$

where the crossover (or saturation) time t^* depends also on the system size

$$t^* \sim L^z. \quad (6)$$

The exponents α , β , and z are linked by the scaling law

$$z = \frac{\alpha}{\beta}. \quad (7)$$

Let us consider first the RD of two annihilating species with the TA rule. Figures 2 and 3 show our simulation results for the average height and the width of the interface, for different values of the probability p and fixed system size L .

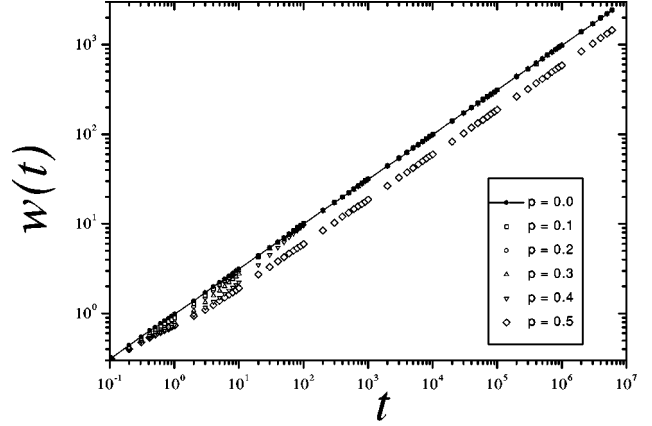


FIG. 3. Log-log plot for the temporal dependence of the interface width $w(t)$ with the TA rule, for various probabilities p and fixed system size $L=75$. The observed value for the growth exponent is $\beta = 0.4994 \pm 0.0002$.

Periodic boundary conditions are used in the horizontal direction, and the statistical average is obtained over 200 independent simulations for each parameter.

Since there is no correlation between columns, every A (or B) column grows independently with probability p (q) and decreases with probability q (p). The probability that a given column has height $h = |N_A - N_B|$ after deposition of $N = N_A + N_B$ particles is given by the binomial distribution, which for $N \rightarrow \infty$ becomes the Gaussian distribution. It is straightforward to prove that the asymptotic behavior is given exactly by

$$\langle h(t) \rangle \sim \begin{cases} |p - q|t, & p \neq q, \\ \left(\frac{2}{\pi} t \right)^{1/2}, & p = q = 1/2, \end{cases} \quad (8)$$

$$w(t) \sim t^{1/2}, \quad 0 \leq p, q \leq 1/2, \quad (9)$$

in agreement with the numerical results and reproducing the same scaling exponents as common RD, $\beta = 1/2$ and $\alpha =$ (not defined), i.e., the interface width increases as $t^{1/2}$, but never saturates. It is clear that the most probable arriving particle will finally cover the whole structure. When $p = q$, the problem is essentially a random walk in the semiaxis $h > 0$ with a reflecting wall at $h = 0$ [14], which gives a nonvanishing average height $\langle h \rangle \sim t^{1/2}$.

Most interesting is the RD of two annihilating species with NNA rule, since it allows the segregation of like particles. Figure 4 shows the average height as a function of time for different values of the probability p and fixed system size L . In this case $\langle h(t) \rangle$ is smaller than that observed in Fig. 2. This fact is expected since with the NNA rule adjacent columns of unlike particles cannot exist, so as p increases a larger number of vacant columns will appear, which reduces the interface height. However, in the limit $t \rightarrow \infty$ we obtain essentially the same asymptotic behavior as in the TA model.

Figure 5 shows the time evolution of the surface width w , for different values of the probability and fixed system size L . Note that the interface width first increases very fast and

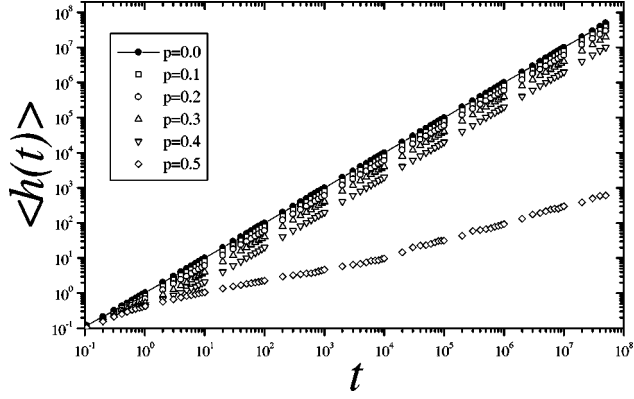


FIG. 4. As in Fig. 2 but here with the NNA rule. The asymptotic slopes are the same as those in Fig. 2.

finally saturates to a constant value which depends on the probability p . In the growth regime the time dependence of the width follows a power law

$$w(p,t) \sim t^{\beta'}, \quad t \ll t'. \quad (10)$$

For $0 < p < 1/2$ we obtain $\beta' \approx 1/2$, and for $p = 1/2$, $\beta' \approx 1/4$. Then the surface width becomes smaller as the probability p increases up to $p = 1/2$. Of course, the behavior is symmetric in p around $p = 1/2$. It is clear that the competition between deposition and reaction leads to saturation. From Fig. 5 we observe that the saturation width $w_{\text{sat}}(p) \equiv w(p, t \rightarrow \infty)$ decreases monotonically with the probability p . The saturated surface width versus the probability p , for fixed values of the system size is shown in Fig. 6. According to this figure, the dependence of the saturated width $w_{\text{sat}}(p)$ on the probability p also follows a power law

$$w_{\text{sat}}(p) \sim p^{\alpha'}, \quad t \gg t', \quad (11)$$

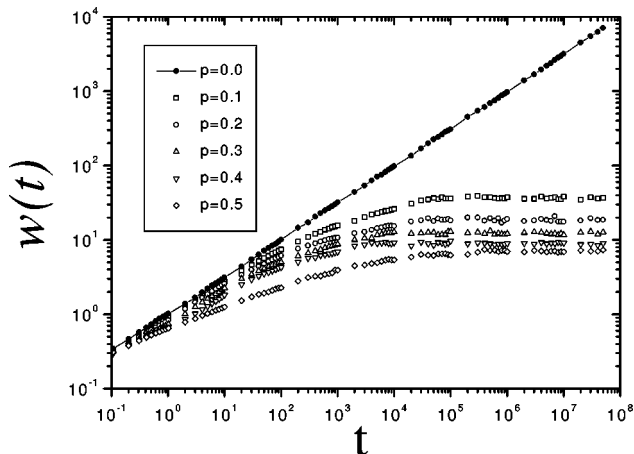


FIG. 5. As in Fig. 3 but here with the NNA rule. The growth exponents are $\beta' = 0.5003 \pm 0.0019$ for $0 < p < 1/2$ and $\beta' = 0.262 \pm 0.004$ for $p = 1/2$.

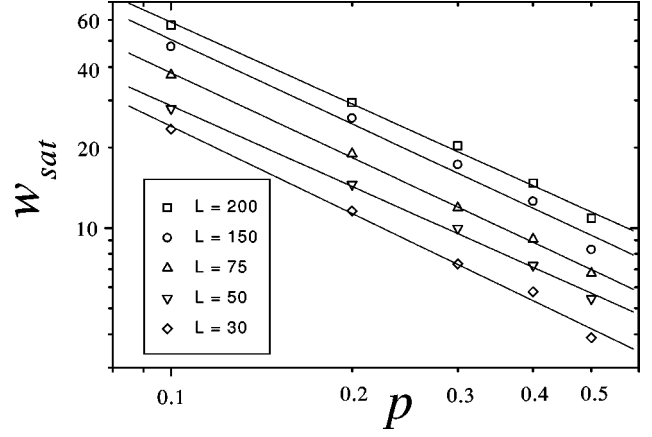


FIG. 6. The saturated widths $w_{\text{sat}}(p)$, as a function of probability p and fixed system size L . The observed value for the exponent in Eq. (11) is $\alpha' = -1.04 \pm 0.08$.

and surprisingly α' is found to be universal, i.e., regardless of the system size L , we obtain $\alpha' \approx -1$. It should be noted that $w_{\text{sat}}(p) \rightarrow \infty$ for $p \rightarrow 0$, in agreement with the common RD model.

It is also interesting to analyze the time dependence of the width w for different values of the size L and fixed probability p , which is shown in Fig. 7. Initially the width increases as a power of time

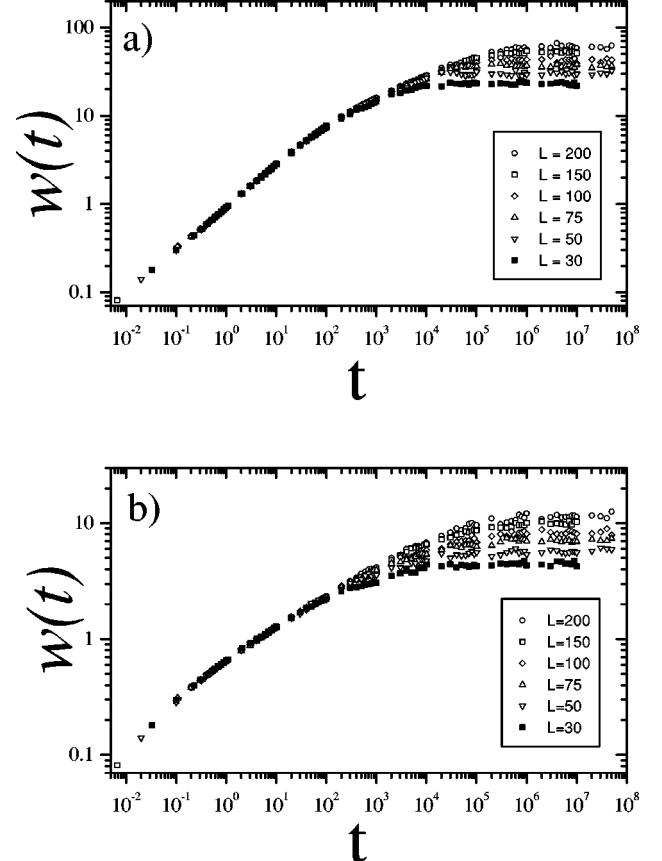


FIG. 7. Log-Log plot for the time dependence of the interface width $w(t)$ with the NNA rule, for different values of the system size L and fixed probabilities (a) $p = 0.1$ and (b) $p = 0.5$.

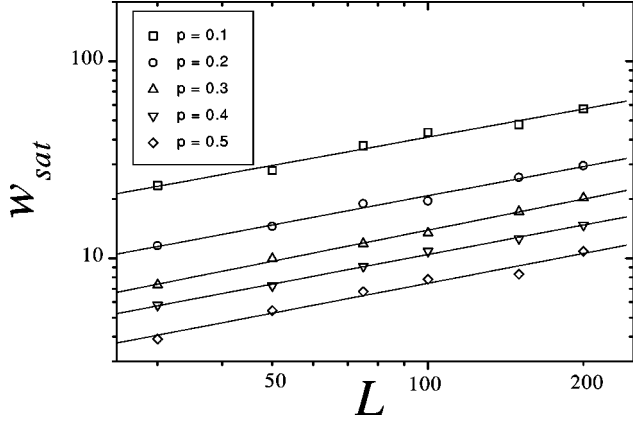


FIG. 8. Log-log plot for the saturated widths $w_{\text{sat}}(L)$, as a function of system size L and fixed probability p . The roughness exponent is $\alpha = 0.497 \pm 0.041$.

$$w(L, t) \sim t^\beta, \quad t \ll t^*, \quad (12)$$

where the growth exponent is observed to be $\beta \approx 1/2$ for $0 < p < 1/2$ and $\beta \approx 1/4$ for $p = 1/2$.

From Fig. 7 it is evident that the saturation width $w_{\text{sat}}(L) \equiv w(L, t \rightarrow \infty)$ increases monotonically with the system size, as in common deposition processes without reaction such as random deposition with relaxation or ballistic deposition (BD). The saturated surface width as a function of the system size L , for fixed values of the probability p , is presented in Fig. 8. Here we again observe a simple power law for the saturated width $w_{\text{sat}}(L)$ with the system size

$$w_{\text{sat}}(L) \sim L^\alpha \quad t \gg t^*, \quad (13)$$

where the roughness exponent is $\alpha \approx 1/2$ independent of the probability p .

Fortunately, there is a simple way to collapse all the data recorded onto a single curve. If we plot $w(L, p, t)/w_{\text{sat}}(L, p)$ as a function of $t/(p^{z'} L^z)$, the result will be a unique curve independent of the system size L and the probability p . Then $w(L, p, t)/w_{\text{sat}}(L, p)$ is a function of $t/(p^{z'} L^z)$ only, and we write

$$\frac{w(L, p, t)}{w_{\text{sat}}(L, p)} \sim f\left(\frac{t}{p^{z'} L^z}\right), \quad (14)$$

where $f(u)$ is a scaling function, $z \equiv \alpha/\beta$, and $z' \equiv \alpha'/\beta' = \alpha'/\beta$.

From Eqs. (11) and (13) we have

$$w_{\text{sat}}(L, p) \sim w_{\text{sat}}(L) w_{\text{sat}}(p) \sim L^\alpha p^{\alpha'}. \quad (15)$$

Then we obtain the scaling relation

$$w(L, p, t) \sim L^\alpha p^{\alpha'} f\left(\frac{t}{p^{z'} L^z}\right). \quad (16)$$

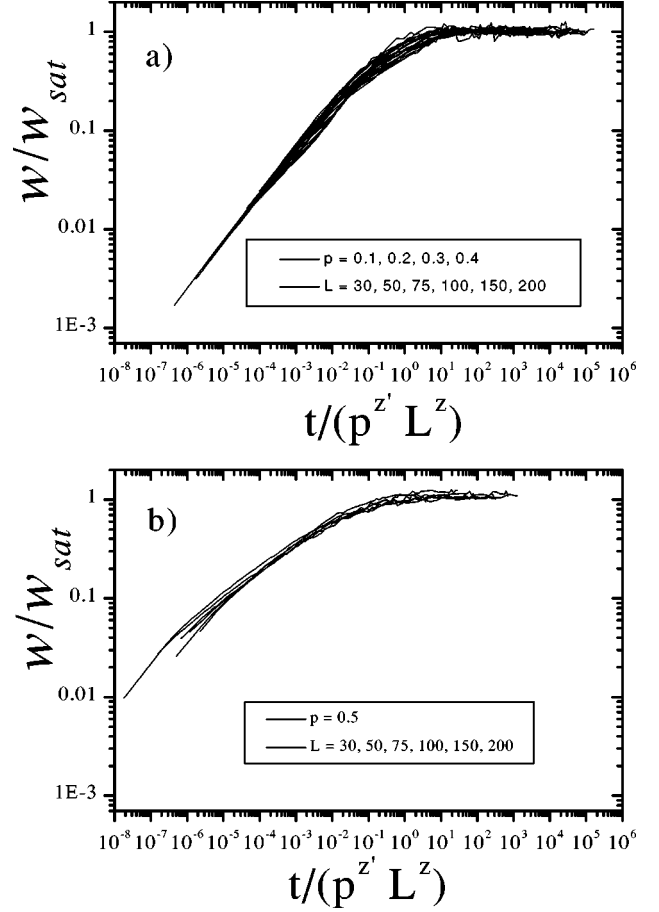


FIG. 9. The random deposition with NN annihilation data rescaled according to Eq. (14). In (a) $0 < p < 1/2$, $\beta = \beta' = 1/2$, $z = 1$, and $z' = -2$. In (b) $p = 1/2$, $\beta = \beta' = 1/4$, $z = 2$, and $z' = -4$.

There are two scaling regimes depending on the argument $u \equiv t/p^{z'} L^z$.

(a) For small u , the scaling function increases as a power law, and we have

$$f(u) \sim u^\beta, \quad u \ll 1. \quad (17)$$

(b) For $t \rightarrow \infty$ the width saturates, and in this limit we have

$$f(u) = \text{const}, \quad u \gg 1. \quad (18)$$

The validity of the scaling assumption (14) is shown in Fig. 9. It should be clear that curves with different values of scaling exponents cannot be collapsed onto a unique and universal curve.

To conclude this paper we address some questions of universality. It is well known that a wide variety of growth models for deposition processes belong to one of the following three different universality classes.

(i) Random deposition with $\beta = 1/2$ and $\alpha =$ (not defined) [15].

(ii) Edwards-Wilkinson (EW), with $\beta = 1/4$ and $\alpha = 1/2$ [16].

(iii) Kardar-Parisi-Zhang (KPZ), with $\beta = 1/3$ and $\alpha = 1/2$ [17].

As was already observed, the case where $p = 0$ is trivial

and reproduces the same scaling exponents as RD. For $p = 1/2$ the values or the scaling exponents are found to be $\beta \approx 1/4$ and $\alpha \approx 1/2$, essentially the same exponents as the EW universality class. However, when $0 < p < 1/2$ the scaling exponents are $\beta \approx 1/2$ and $\alpha \approx 1/2$, which do not belong to any of the above universality classes. This situation could be interpreted as a crossover or hybridization between RD and EW universality classes. Another remarkable result is the universality of the exponent α' in Eq. (11). Clearly one expects that w_{sat} should depend on p , but it is not intuitively

obvious that such a dependence is a simple power law with as well a well defined exponent as that of Eq. (11). Future efforts will be directed to studying the same problem in a two-dimensional substrate and obtaining a partial differential equation describing the evolution of the interface.

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