Front propagation and diffusion in the A⇆A+A hard-core reaction on a chain

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Front propagation and diffusion in the $A \leftrightarrows A+A$ hard-core reaction on a chain

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We study front propagation and diffusion in the reaction-diffusion system $A \leftrightarrows A+A$ on a lattice. On each lattice site at most one A particle is allowed at any time. In this paper, we analyze the problem in the full range of parameter space, keeping the discrete nature of the lattice and the particles intact. Our analysis of the stochastic dynamics of the foremost occupied lattice site yields simple expressions for the front speed and the front diffusion coefficient which are in excellent agreement with simulation results.

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I. INTRODUCTION

In this paper, we study the propagation and diffusion of a *front* in the $A \leftrightarrows A+A$ reaction on a chain, in the case that there cannot be more than one A particle on each lattice site (''hard-core exclusion''). The front propagation problem we consider is the following. We start from a situation illustrated in Fig. 1(a) in which there are no A particles at all on the right half of the system, while there is a nonzero density of particles on the left. The object of study is then the asymptotic average speed v with which the region with a nonzero density of particles expands to the right, as well as the effective diffusion coefficient D_f of this ''front.'' For the hard-core exclusion problem, the front position is most conveniently defined as the position of the foremost (rightmost) particle, see Figs. 1(a,b). The average front speed and front diffusion coefficient are then the average drift speed v and the diffusive spreading $\sim \sqrt{D_f t}$ of the width of the probability distribution $P_{k_f}(t)$ for the location k_f of the foremost occupied lattice site, as illustrated in Fig. 1(c). One of the main results of the paper is a simple expression for v and D_f, which is accurate in the range where the deviations from the mean-field theory are large. Our results reduce to an exact expressions derived before for the particular case in which the particle diffusion coefficient D and annihilation rate W are equal [1] and our expression for the front speed v reduces to the approximate expression obtained for the special case $W=0$ in Refs. [2–4]. In addition, we study the average particle profile behind the foremost occupied lattice site and analyze how its behavior affects the average front speed and diffusion.

The perspective of this work lies in the issues that have emerged from the surprising findings for fronts in this reaction-diffusion system in the limit in which N, the average number of particles per lattice site in equilibrium, is large. In a lattice model, one can tune N by allowing more than one particle per site (no hard-core exclusion) and changing the ratio k_b/k_d, where k_b is the reaction rate for birth processes $A \to 2A$ and k_d the reaction rate for death processes, $2A \to A$, as the average equilibrium number of particles $N = k_b/k_d$. In the limit $N \to \infty$, the normalized particle density $\rho_i \equiv N_i/N$ then obeys a mean-field equation which is a lattice analog of the continuum reaction-diffusion equation $\partial_t \rho = D\partial_x^2 \rho + \rho - \rho^2$, where D is the diffusion rate of individual particles on the chain. The front problem mentioned above, i.e., the propagation of a front into an empty region, then corresponds in the mean-field limit $N \to \infty$ to a front propagating into the linearly unstable state $\rho = 0$ (the mean-field behavior is also obtained in the limit in which the particle diffusion coefficient $D \to \infty$ [2–4], but we will focus on the case in which the diffusion coefficient is finite and comparable to the growth and annihilation rates). The behavior of such fronts in deterministic continuum equations has been studied since long and is very well understood (see, e.g., Refs. [5,6]). Since the nonlinear front solutions are essentially ''pulled along'' by the growth of the leading edge where $\rho \ll 1$, such fronts are often referred to as *pulled* fronts [6]. The remarkable discovery of the last few years has been that since the propagation is driven by the region where ρ is small, they are particularly sensitive to the discrete nature of the particles which manifests itself in changes in the dynam-

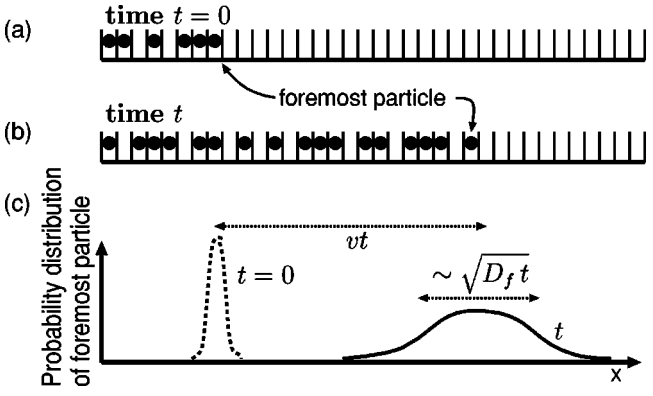

FIG. 1. (a) The type of initial condition we consider for our stochastic model. (b) Illustration of a typical snapshot of the state of the system at finite time. The foremost particle has advanced to the right relative to the one where it started at $t=0$. (c) Qualitative sketch of the probability distribution function for the foremost particle at $t=0$ (dashed line) at large times t; the center of the peak drifts with speed v, while the peak widens proportional to $\sqrt{D_f t}$.

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ics when ρ becomes of order $1/N$. Indeed, Brunet, and Derrida discovered that the convergence to the mean-field limit is extremely slow with N: the average front speed v converges as $1/\ln^2 N$ to the mean-field value [7]. This is in contrast to the fact that for pushed fronts, the convergence to asymptotic speed behaves as a power of $1/N$. This slow convergence has been confirmed for a variety of models [7–14]. In addition, in a model that Brunet and Derrida studied in Ref. [8], the front diffusion coefficient D_f was numerically shown to vanish only as $1/\ln^3 N$.

The dominant asymptotic correction to the mean-field result for the front speed in the limit $N\to\infty$ traces simply to the change in the dynamics at $\rho = O(1/N)$ [7], and as a result appear to be universal. However, all corrections beyond the asymptotic one appear to depend *nonuniversally* on the detailed stochastic dynamics at the foremost occupied site and those closely behind it, where asymptotic techniques are of no use since the number of particles involved in the dynamics is small [14]. Moreover, the stochastic dynamics in the tip region even seems to be strongly nonlinearly coupled to the uniformly translating average front profile behind the tip.

For analyzing these effects for finite values of the particle diffusion coefficient D and particle number N, it is found to be expedient to develop a stochastic front description by focussing on the behavior of the foremost particle or the foremost occupied bin [14]. As it turns out, this idea traces back to the earlier work by Kerstein [2,4], and Bramson and coworkers [3]. These authors analyzed the average front speed v for a special case of the model we investigate here, namely, the case in which the particle annihilation rate $W=0$. In this case, one can formulate a self-consistent dynamics for the two foremost particles [15], but this important simplification is lost when $W\neq 0$ [16]. Motivated by the desire to understand the ingredients necessary to analyze the stochastic front behavior for finite values of D, W, and N, we focus here on analyzing both v and D_f in the case in which all the transition rates are comparable; our analysis includes the special point $D=W$ where an exact result was obtained by ben-Avraham [1].

II. THE MODEL, FRONT SPEED, AND FRONT DIFFUSION

We now turn to the details of our model and our results for the stochastic fronts. We consider a chain on which A particles can undergo the following three basic moves, shown in Fig. 2:

(a) A particle can diffuse to any one of its neighbor lattice sites with a diffusion rate D, provided this neighboring site is empty.

(b) Any particle can give birth to another one on any one of its empty neighbor lattice sites with a birth rate ε.

(c) Any one of two A particles belonging to two neighboring filled lattice sites can get annihilated with a death rate W.

Note that in the above formulation, diffusive hops to neighboring sites which are occupied are not allowed. We can also think about these stochastic moves differently: for example, we can allow nearest neighbor diffusive hops to a site which is already occupied be followed by an instantaneous annihilation of one of the two particles. If we do so, then the diffusive process contributes to the annihilation of particles. However, in this paper we shall stick to the convention that diffusive hops are allowed only to empty sites.

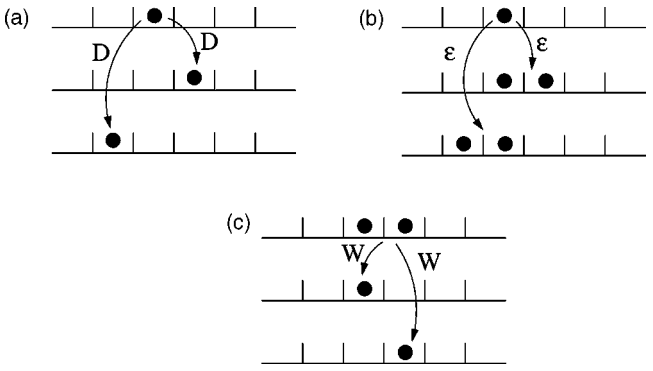

FIG. 2. The microscopic processes that take place inside the system: (a) a diffusive hop with rate D to a neighboring empty site; (b) creation of a new particle on a site neighboring an occupied site with rate ε; (c) annihilation of a particle on a site adjacent to an occupied site at a rate W.

As noted before, earlier work on models of this type includes that of Kerstein [2,4] and Bramson *et al.* [3] on the case $W=0$ and that of ben-Avraham on the case $D=W$ [1] (also, variants of this model have been analyzed in Refs. [17–19]). Notice that in the general case there are essentially only two nontrivial parameters in the model, e.g., the ratios D/ε and D/W, since an overall multiplicative factor just sets the time scale. Our interest is in the parameter range where both of these ratios are $\mathcal{O}(1)$; when these ratios tend to infinity, the front speed approaches the mean-field value [2–4].

For an ensemble of front realizations, let us denote the probability distribution for the foremost occupied lattice site to be at lattice site k_f by $P_{k_f}(t)$. The evolution of $P_{k_f}(t)$ is then described by

$$\frac{dP_{k_f}}{dt} = (D+\varepsilon)P_{k_f-1} + [DP^{\rm empty}_{k_f+1} + WP^{\rm occ}_{k_f+1}] - (D+\varepsilon)P_{k_f} - [DP^{\rm empty}_{k_f} + WP^{\rm occ}_{k_f}]. \quad (1)$$

Here, $P^{\rm occ}_{k_f}(t)$ and $P^{\rm empty}_{k_f}(t)$ denote the joint probabilities that the foremost particle is at site k_f and that the site k_f-1 is occupied or empty, respectively. Clearly, $P_{k_f}(t) = P^{\rm occ}_{k_f}(t) + P^{\rm empty}_{k_f}(t)$, and $\Sigma_{k_f} P_{k_f}(t) = 1$. The first term on the right-hand side of Eq. (1) describes the increase in $P_{k_f}(t)$ due to the advancement of a foremost occupied lattice site from position k_f-1, while the second term describes the increase in $P_{k_f}(t)$ due to the retreat of a foremost occupied lattice site from position k_f+1. The third and the fourth terms, respectively, describe the decrease in $P_{k_f}(t)$ due to the advancement and retreat of a foremost occupied lattice site from position k_f.

From the definition of $P_{k_f}(t)$, the mean position and the width of the distribution for the positions of the foremost occupied lattice sites are defined as $x(t)=\Sigma_{k_f} k_f P_{k_f}(t)$ and $\langle \Delta x^2(t)\rangle = \Sigma_{k_f}[k_f - x(t)]^2 P_{k_f}(t)$ [20]. The mean speed and diffusion coefficient of the front are thus given in terms of these quantities as the $t\to\infty$ limit of $v=dx(t)/dt$ and $\langle \Delta x^2(t)\rangle = 2D_f t$—see Fig. 1(c). To obtain them, we need the expressions of $P^{\rm occ}_{k_f}(t)$ and $P^{\rm empty}_{k_f}(t)$. To start with, we have

$$P^{\rm occ}_{k_f}(t) = \rho_{k_f-1} P_{k_f}(t), \tag{2}$$

where ρ_{k_f-1} is the conditional probability of having the (k_f-1)th lattice site occupied (the foremost particle is at the k_fth lattice site). The set of conditional occupation densities ρ_{k_f-m} for $m \geqslant 1$ can be thought of as determining the front profile in a frame moving with each front realization. For obtaining v and D_f, we simply need to know the asymptotic long-time limit $\rho_{k_f-1}(t\to\infty)$, which from here on we will denote simply as ρ_{k_f-1}. Given ρ_{k_f-1}, it is then straightforward to obtain from Eq. (1) and the conditions $P_{k_f}(t) = P^{\rm occ}_{k_f}(t) + P^{\rm empty}_{k_f}(t)$ and $\Sigma_{k_f} P_{k_f}(t) = 1$,

$$v = \frac{dx}{dt} = \varepsilon - \rho_{k_f-1}(W-D)$$

and

$$\frac{d\langle \Delta x^2\rangle}{dt} = 2D + \varepsilon + \rho_{k_f-1}(W-D). \tag{3}$$

Of these, the second equation indicates that the front wandering is diffusive, and an expression of the front diffusion coefficient D_f is therefore given by

$$D_f = \frac{1}{2}[2D + \varepsilon + \rho_{k_f-1}(W-D)]. \tag{4}$$

As noted already by ben-Avraham [1] in a continuum formulation of the present model, for the special case $D=W$ the unknown quantity ρ_{k_f-1} drops out of Eq. (3); it thus leads to the *exact* results $v=\varepsilon$ and $D_f = D + \varepsilon/2$ as a special cases of Eq. (4) for $D=W$. We also note that if we use Eq. (2) in Eq. (1), the latter equation has the form of the master equation for a single random walker on a chain. Thus, we can think of the foremost particle as executing a biased random walk, and D_f as the effective diffusion coefficient of this walker. Moreover, if we eliminate ρ_{k_f-1} from Eqs. (3) and (4), we get the following *exact* relation:

$$v/2 + D_f = D + \varepsilon. \tag{5}$$

In order to obtain an explicit prediction for v and D_f, we need an expression for ρ_{k_f-1}. Far behind the front the particle density will approach the homogeneous equilibrium density $\overline{\rho}$: $\lim_{m\to\infty}\rho_{k_f-m} = \overline{\rho}$. From the master equation it is easy to show that the homogeneous equilibrium solution for the total probability is of product form (so that the probability of having different sites is occupied is uncorrelated), and that the equilibrium occupation density $\overline{\rho}$ is simply given by $\overline{\rho} = \varepsilon/(\varepsilon + W)$.

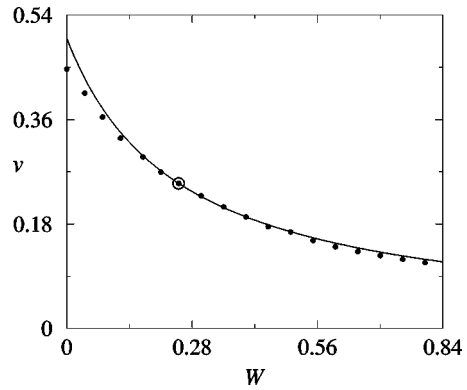

FIG. 3. Comparison of the expression of v in Eq. (6) (solid line) with stochastic simulation data (filled circles), for $D=\varepsilon=0.25$. The error in the data is of the order of the size of the symbols. The corresponding data point for $D=W$, as analyzed in Ref. [1], is shown by the larger open circle.

The crudest approximation for the front profile ρ_{k_f-m}, and, in particular, for ρ_{k_f-1} is to just take $\rho_{k_f-1} \approx \overline{\rho}$. Substitution of this approximation into Eqs. (3) and (4) immediately yields our main result,

$$v = \frac{\varepsilon(\varepsilon+D)}{\varepsilon+W} \quad \text{and} \quad D_f = \frac{(\varepsilon+2W)(D+\varepsilon)}{2(\varepsilon+W)}. \tag{6}$$

For $W=0$, the expression for v reduces to the one obtained in Refs. [2–4].

In what follows, we will first compare these approximate expressions for v and D_f to the results of computer simulation for the case $D/\varepsilon = 1$ [21], and then investigate the appropriateness and shortcomings of the approximation $\rho_{k_f-1} \approx \overline{\rho}$.

The comparison of Eq. (6) with stochastic simulation data for $D=\varepsilon=0.25$ are presented in Figs. 3 and 4 as a function

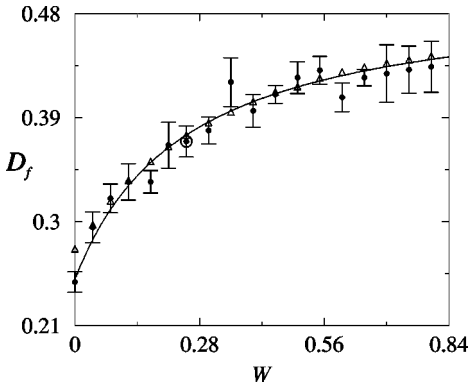

FIG. 4. Comparison of the front diffusion coefficient according to Eq. (6) (solid line) with stochastic spreading data (filled circles) and with Eq. (5) (open triangles), for $D=\varepsilon=0.25$. The large open circle once again corresponds to the direct measurement of the effective front diffusion coefficient for $D=W$, as analyzed in Ref. [1].

of W for $D=\varepsilon=0.25$. The simulation algorithm has been adopted from Ref. [14], and is essentially the same one as in Ref. [9]. The speed v has been obtained directly from the average position of the foremost occupied lattice site in a single long run according to $v(t)=[x(t)-x(t_0)]/(t-t_0)$ corresponding to $x(t)-x(t_0)=15\,000$ consecutive forward jumps. The diffusion coefficient has been determined both from the speed measurements via Eq. (5) and from data for the average diffusive spreading during 1000 time intervals Δt up to 500 taken from five long runs (of which the data from the first 5000 consecutive forward jumps of the foremost occupied lattice site were ignored, so as to eliminate initial transient effects). For each of these runs, the mean square displacement $\langle \Delta x^2 \rangle$ was confirmed to grow linearly with time. Figures 3 and 4 show that our approximate expressions (6) for the speed and diffusion coefficient (solid line) are quite accurate for $D/\varepsilon=1$ over the whole range of values of W where we have performed simulations; interestingly, the values of D_f obtained from the speed measurements via Eq. (5) are more accurate than those obtained directly from the diffusive spreading. The error bars in Fig. 4 correspond to the standard deviations of D_f values obtained from five long runs.

We now return to the issue of the appropriateness of the assumption $\rho_{k_f-1}=\overline{\rho}$. While the agreement between the theoretical prediction for v and D_f gives empirical evidence that this assumption is a reasonably good one, we see from Fig. 3 that although Eq. (6) agrees well with the simulation data, there are small but systematic deviations on both sides of this region. These deviations can be explained as follows: As $W \to 0$, $\overline{\rho} \uparrow 1$; far behind the front all lattice sites are occupied. However, the density of particles just behind the foremost one is smaller, since it takes a finite time for the density to relax to the asymptotic one. For large values of W, the effective diffusion rate is much larger than the drift rate, as Eq. (6) shows. As a result, once again the density of particles just behind the foremost one also has relatively small time to relax to the asymptotic value. This is reflected in the difference between ρ_{k_f-1} and $\overline{\rho}$ in Fig. 5.

The above trends are borne out by the simulation results of Fig. 5, where we plot the relative deviation $d=(\rho_k-\overline{\rho})/\overline{\rho}$ for $k=k_f-1,\ldots,k_f-6$. First of all, the data confirm that unless the value W is too small, $\rho_{k_f-1}=\overline{\rho}$ is quite a good approximation, and that the density behind the foremost particle is enhanced for large W and reduced for small W. We also note that we have verified that if one substitutes the ρ_{k_f-1} values for $W=0$ and $W=0.8$ from Fig. 5 into Eq. (1), one does recover the corresponding measured speeds, as one should.

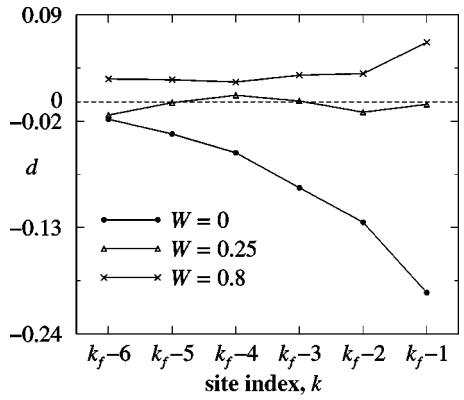

FIG. 5. Relative deviation $d=(\rho_k-\overline{\rho})/\overline{\rho}$ of the average density from $\overline{\rho}=\varepsilon/(\varepsilon+W)$ for the first six lattice sites to the left of the foremost occupied lattice site k_f for $D=\varepsilon=0.25$ and three different values of W.

III. CONCLUSION

In conclusion, this work clearly illustrates that the concept of the dynamics of the foremost occupied lattice site, in Refs. [2–4,14] and here, can be a viable route towards analyzing the front propagation and diffusion in stochastic lattice models. In the present $N \leqslant 1$ model a simple approximation for the interaction of the foremost particle with the front region behind it already yields quite accurate results for v and D_f. We hope that this success provides new motivation and inspiration to tackle the complicated case in which N is large but finite.

In principle, it should be possible to extend the analysis in the spirit of the one developed by Kerstein [2,4] to get successively more accurate expressions for ρ_{k_f-1}, and correspondingly for the front speed and diffusion coefficient. In particular, such extensions might allow one to use the results in a wider parameter range, such as $D/W \to \infty$ while $D/\varepsilon \sim O(1)$, or $D/\varepsilon \to \infty$ while $W/\varepsilon \sim O(1)$. However, inspection of the earlier analysis suggests that such higher order analytical expressions of ρ_{k_f-1} are less trivial to obtain than one might expect at first sight. More precisely, in the light of Refs. [15,16], it is clear that for $W \neq 0$, the master equation for the probability that the two foremost particles are separated by k lattice sites couples to probability distributions involving particles that are further back. While it is certainly possible to solve the master equation numerically, it does not appear to lead one to an analytical expression of ρ_{k_f-1} that provides a better approximation than what we have used in this paper.

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[1] D. ben-Avraham, Phys. Lett. A **247**, 53 (1998).
[2] A.R. Kerstein, J. Stat. Phys. **45**, 921 (1986).
[3] M. Bramson, P. Calderoni, A. De Masi, P.A. Ferrari, J.L. Lebowitz, and R.H. Schonmann, J. Stat. Phys. **45**, 905 (1986).
[4] A.R. Kerstein, J. Stat. Phys. **53**, 703 (1988).
[5] D.G. Aronson and H.F. Weinberger, Adv. Math. **30**, 33 (1978).
[6] U. Ebert and W. van Saarloos, Physica D **146**, 1 (2000).
[7] E. Brunet and B. Derrida, Phys. Rev. E **56**, 2597 (1997).

[8] E. Brunet and B. Derrida, J. Stat. Phys. **103**, 269 (2001).
[9] H.P. Breuer, W. Huber, and F. Petruccione, Physica D **73**, 259 (1994).
[10] R. van Zon, H. van Beijeren, and Ch. Dellago, Phys. Rev. Lett. **80**, 2035 (1998).
[11] D.A. Kessler, Z. Ner, and L.M. Sander, Phys. Rev. E **58**, 107 (1998).
[12] L. Pechenik and H. Levine, Phys. Rev. E **59**, 3893 (1999).
[13] D. Panja and W. van Saarloos, Phys. Rev. E **65**, 057202 (2002); **66**, 015206 (2002).
[14] D. Panja and W. van Saarloos, Phys. Rev. E **66**, 036206 (2002).
[15] As can be seen from Eqs. (3), to obtain the front speed and the front diffusion coefficient, one needs the expression of ρ_{k_f-1}, the probability of the occupancy of the lattice site just behind the foremost particle. For $W=0$, the ''two-particle self-consistent'' approach developed in Refs. [2,4] can obtain a better approximation of ρ_{k_f-1} than what we present in this paper, from the solution of the master equation for the probability that the two foremost particles are separated by k lattice sites.
[16] For $W=0$, the master equation for the probability that the two foremost particles are separated by k lattice sites can be closed in a simple manner [2,4]. In this formalism, no particle gets annihilated, and as a result, the hierarchy of equations for the joint probability density distribution of the two foremost particles can be closed easily at the simplest level, since in the absence of annihilation, the third foremost particle never becomes the second foremost particle. At this level, the expression of ρ_{k_f-1} can then be analytically solved, leading to a better approximation than what we use in this paper for $W=0$. Of course, the master equation can be closed at a higher level, by considering more than two foremost particles to determine ρ_{k_f-1}, but then one does not obtain an analytical expression of ρ_{k_f-1}. As soon as $W\neq 0$, this is not true anymore: consider the following situation where the two foremost particles are next to each other. With annihilation of particles allowed, one of them can annihilate the other, and then the probability distribution function of the two foremost particles is crucially coupled to those which involve particles further back at the simplest level.
[17] D. ben-Avraham, M.A. Burschka, and C.R. Doering, J. Stat. Phys. **60**, 695 (1990).
[18] C.R. Doering, M.A. Burschka, and W. Horsthemke, J. Stat. Phys. **65**, 953 (1991).
[19] C.R. Doering, Physica A **188**, 386 (1992).
[20] One can also define the foremost occupied lattice site for a realization as the one on the right of which no lattice site has ever been occupied before, and obtain the front speed from this definition following [14]. Both of them, of course, yield the same result due to the $t\rightarrow\infty$ limit.
[21] We note here that the choice of $D/\varepsilon=1$ is only coincidental, and the relative agreements in Figs. 3 and 4, are not affected so long as D and ε are of the same order of magnitudes.