Effect of Microscopic Noise on Front Propagation

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We study the effect of the noise due to microscopic fluctuations on the position of a one dimensional front propagating from a stable to an unstable region in the "linearly marginal stability case." By simulating a very simple system for which the effective number N of particles can be as large as $N = 10^{150}$, we measure the N dependence of the diffusion constant D_N of the front and the shift of its velocity v_N. Our results indicate that $D_N \sim (\log N)^{-3}$. They also confirm our recent claim that the shift of velocity scales like $v_{\min} - v_N \simeq K(\log N)^{-2}$ and indicate that the numerical value of K is very close to the analytical expression K_{approx} obtained in our previous work using a simple cut-off approximation.

1. INTRODUCTION

Fronts propagating from a stable region into an unstable region appear in many different contexts in physics, chemistry or biology.[1–8] These fronts are usually described at the macroscopic level by equations of the type of the Fisher-KPP equation (KPP = Kolmogorov, Petrovsky, Piscounov):[1, 2]

$$\frac{\partial h}{\partial t} = \frac{\partial^2 h}{\partial x^2} + h - h^2 \tag{1}$$

where $0 \leqslant h(x, t) \leqslant 1$. This equation was first used to describe the spread of an advantageous gene in a population; $h(x, t)$ is then the space- and time-dependent proportion of the population with the favorable gene.

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It is well known$^{(9-11, 5)}$ that a large class of equations describing the propagation of a front into an unstable region and known as the "linearly marginal stability case"$^{(12)}$ or the "pulled case"$^{(5)}$ have properties similar to (1): these equations admit a continuous family of propagating front solutions

$$h(x, t) = F_v(x - vt) \tag{2}$$

for any velocity v larger than a minimal velocity v_{min}, and the front moves with this minimal velocity v_{min} for steep enough initial conditions (that is, when $h(x, 0)$ decays fast enough as $x \to \infty$). For Eq. (1), this minimal velocity is $v_{min} = 2$.

These noiseless equations usually represent a mean field description of some microscopic reaction diffusion processes.$^{(13)}$ Many approaches have been proposed to try to understand the corrections to this mean field picture due to the stochastic aspect present at the microscopic level.

Some approaches add a multiplicative noise term to the equation in a phenomenological way,$^{(14-17)}$ but the noise term introduced that way represents an external noise and not the fluctuations of the underlying microscopic model. Other approaches use a mesoscopic description$^{(18-22)}$ (using Boltzmann or Langevin equations) or attack directly the microscopic model,$^{(23-27)}$ but the effective numbers N of particles which can be numerically achieved are usually too small to see the large N behavior in the one dimensional case.

What has become clear, however, over the last fifteen years is that:

• In contrast to the macroscopic equations which admit a continuous family of solutions, a single velocity is selected by the front in the microscopic models for arbitrary initial conditions.$^{(13, 28, 23, 24, 18, 19, 27)}$

• This velocity is smaller than v_{min} and tends slowly to v_{min} as $N \to \infty$ (i.e., as one approaches the mean field limit).$^{(13, 28, 23, 24, 29-33)}$

• The front has a fluctuating shape but its width does not broaden with time.$^{(27, 34)}$

• The position of the front diffuses with time$^{(23, 24, 35, 34)}$ with a diffusion constant D_N which decreases slowly with N.

Only recently, by considering simple enough one dimensional lattice models,$^{(29-33)}$ it was possible to increase N (or the effective N) enough to see that the velocity of the front v_N, for microscopic models, converges to v_{min} from below with a correction proportional to $1/\log^2 N$.

$$v_N - v_{min} \simeq -\frac{K}{\log^2 N} \tag{3}$$

A simple approximation (*the cut-off approximation*) developed in ref. 29 predicts this logarithmic correction together with an analytic expression K_{approx} for the multiplicative constant K in (3). (In the case of Eq. (1), it gives $K_{\text{approx}} = \pi^2$.) This approximation is simply based on the idea that the concentration $h(x, t)$ is quantized at the microscopic level and varies by steps of $1/N$ without any reference to the stochastic nature of the microscopic model.

Simulations indicate[29, 30] that the cut-off approximation gives the right order of magnitude for K but it is still not established[33] whether $K = K_{\text{approx}}$ or not.

The main goal of the present paper is to give numerical evidence that the diffusion constant D_N has also a logarithmic decay for large N

$$D_N \simeq \frac{K'}{\log^\alpha N} \tag{4}$$

with $\alpha = 3 \pm 0.1$. We have at present no analytical theory to predict K' or α.

Moreover, our numerical simulations confirm the recent results of Pechenik and Levine[33] on a different model, namely that the true value K in (3) is very close and possibly equal to the prediction K_{approx} of the cut-off approximation.

Our paper is organized as follows: in Section 2, we define our microscopic model which is a variant of the model we considered in our previous work[29] and we summarize the analytical results published there. In Section 3, using effective values of N as large as 10^{150}, we present our new results for the velocity v_N and the diffusion constant D_N. Finally, in Section 4 we introduce a simplified version of the model, where the noise is limited to a single site at the tip of the front. The large N behavior of this simplified model cannot be distinguished numerically from the large N behavior of the microscopic model of Sections 2 and 3.

2. THE MICROSCOPIC STOCHASTIC MODEL

2.1. Definition of the Model

The model we study here is a close variant of the one we studied in ref. 29: we consider a system of N particles moving on a line. Both the time t and the positions $X_1(t), ..., X_N(t)$ of the particles are integers.

Given the positions $\{X_k(t)\}$ of the N particles at time t, their new positions at time $t + 1$ are determined in the following way: for each k between 1 and N, we choose two particles i and i' at random among the

N particles. Each $X_k(t+1)$ is then given by the position of the rightmost of these two particles at time t, plus some noise $\alpha_k(t+1)$

$$X_k(t+1) = \max[X_i(t), X_{i'}(t)] + \alpha_k(t+1) \tag{5}$$

At each time step, the particles i and i' are chosen independently at random (so i and i' depend both on k and on t), and the noise $\alpha_k(t+1)$ is also chosen at random according to

$$\alpha_k(t+1) = \begin{cases} 0 & \text{with probability } 1-p \\ 1 & \text{with probability } p \end{cases} \tag{6}$$

This model was considered in the context of the mean-field theory of directed polymers in a random medium:[36] the quantity $-X_k(t)$ was then the groundstate energy of a directed polymer of length t ending at site k in a randomly connected lattice. One can also think of (5) as a simple model for the evolution of the fitness $X_k(t)$ of an individual in a population with sexual reproduction: for each individual k at generation $t+1$, we choose at random two parents from the previous generation t, and the fitness of the new individual is given by the fitness of its best parent plus a random contribution $\alpha_k(t+1)$ due to mutations.

The N particles evolving according to (5) form a bound state. This can be understood intuitively by a simple argument which shows that it is very unlikely to find the particles grouped in more than a single cluster. Assume that, at time t, the N particles form two clusters far apart, with $N\lambda$ particles in the leftmost cluster and $N(1-\lambda)$ particles in the rightmost one. If N is large enough, at time $t+1$, the most probable number of particles will be $N\lambda^2$ in the leftmost cluster and $N(1-\lambda^2)$ in the rightmost cluster. Therefore, with high probability, the leftmost cluster will loose particles at each time step until it disappears completely.

The N particles therefore form a single cluster and one can interpret the motion of this cluster as a front. Let $h(x, t)$ be the fraction of particles strictly at the right of x:

$$h(x, t) = \frac{1}{N} \sum_{X_k(t) > x} 1 \tag{7}$$

Obviously, $h(x, t)$ is a decreasing function with $h(-\infty, t) = 1$ and $h(+\infty, t) = 0$. Given $h(x, t)$, i.e., given the positions of the N particles at time t, the mean value of $h(x, t+1)$ is the probability that $X_k(t+1) > x$ for any given particle k. Using (5), we find easily

$$\langle h(x, t+1) \mid \{h(x, t)\} \rangle = 1 - p[1 - h(x-1, t)]^2 - (1-p)[1 - h(x, t)]^2 \tag{8}$$

2.2. The Deterministic Equation

When N is very large, the law of large numbers tells us that $h(x, t+1) \simeq \langle h(x, t+1) \rangle$. Thus, the evolution of $h(x, t)$ for the stochastic model (5) reduces to the deterministic equation

$$h(x, t+1) = 1 - p[1 - h(x-1, t)]^2 - (1-p)[1 - h(x, t)]^2 \qquad (9)$$

This equation, discrete in space and time, describes the propagation of a front from a stable region ($h = 1$) into a linearly unstable region ($h = 0$). When $0 < p < 0.5$, the traveling-wave solutions decay exponentially in the region where $h(x, t) \ll 1$:

$$h(x, t) \propto e^{-\gamma(x - v(\gamma) t)} \qquad (10)$$

and one can relate the velocity $v(\gamma)$ of the front to the exponential decay γ of the solutions by using (10) into the linearized version of (9),

$$h(x, t+1) \simeq 2ph(x-1, t) + 2(1-p) h(x, t) \qquad (11)$$

One finds

$$v(\gamma) = \frac{1}{\gamma} \log[2pe^{\gamma} + 2(1-p)] \qquad (12)$$

As for the Fisher-KPP equation (1), the front moves with the minimal velocity $v_{\min} = \min_{\gamma} v(\gamma)$ for steep enough initial conditions.

2.3. The Cut-Off Approximation

When N is large but finite, $h(x, t)$ is quantized and varies by steps of $1/N$: in particular the smallest non-zero value it can take is $1/N$. As the speed of the front is determined by its tail, this cut-off has a strong influence on the propagation of the front. We have studied the effect of this cut-off in ref. 29 by modifying (9) in such a way that $h(x, t+1)$ is set to zero whenever the right hand side of (9) is smaller than $1/N$. We have shown that, due to this cut-off, the velocity v_N of the front becomes smaller than $v_{\min}$ and that the shift in velocity is logarithmic in N. We could calculate analytically the leading correction:

$$v_{\min} - v_N \simeq \frac{K_{\text{approx}}}{\log^2 N} \qquad (13)$$

with K_{approx} given by

$$K_{\text{approx}} = \frac{\pi^2 \gamma^{*2} v''(\gamma^*)}{2} \tag{14}$$

where $v(\gamma)$ is given by (12) for our model and where γ^* is the value of γ for which $v_{\min} = v(\gamma^*)$. Expressions (13, 14) are independent of the precise prescription used to introduce the cut-off.

3. NUMERICAL RESULTS

3.1. Implementation details

The main advantage of the model we consider here is that it allows to simulate systems involving a very large number N of particles. This is due to the fact that the N positions of the particles are integers and one can simulate directly the number of particles (or equivalently $h(x, t)$) at each site x. As the number of non-empty sites increases typically like $\log N$, the reduction in computer time is tremendous.[29]

Using this "parallel" algorithm and an implementation of the binomial distribution found in the numerical recipes,[37] we could in ref. 29 simulate systems with up to 10^{16} particles and measure the velocity v_N accurately enough to observe that the difference $v_{\min} - v_N$ decays like $1/\log^2 N$. However, in order to distinguish between several possible logarithmic decay laws for the diffusion constant D_N and to check whether K_{approx} is possibly equal to K or not, we found it necessary to go beyond 10^{16} particles. Consequently, we present in this paper numerical results with N up to 10^{150} particles.

For such large numbers, the generator of binomial random numbers used in ref. 29 does not work. Instead of doing the hard work of designing a new implementation adapted to these large numbers, we used an approximation of the binomial distribution when the numbers involved become larger than 10^7: we used Poisson deviates to approximate the two tails of the binomial distribution and Gaussian deviates in the bulk. For values of N up to 10^{14}, we compared the results obtained with this approximate distribution to results obtained with the exact binomial distribution, and we could not see any difference between the two sets of results.

Our simulations were done as follows: at time $t = 0$, all the particles are put on the same lattice site $x = 0$, and we measure at each time step the

position of the front by taking the average position of the particles. To obtain the front velocity and the diffusion constant for each choice of the parameters, we first let the system evolve for a certain number T of time-steps to eliminate transient effects due to initial conditions. Then, we measure by how much the front moves during the following $5T$ time-steps and again during the next $50T$ time-steps. Averaged over a large number of runs (more than 1000), these data allow us to estimate the average speed v_N and diffusion constant D_N of the front for the two different time intervals $5T$ and $50T$. The fact that the results for v_N and D_N were the same for the two time intervals was our way to check that the transient effects have actually been suppressed and that the wandering of the front position is indeed diffusive.

It is expected[30] that the relaxation time of the system scales like $\log^2 N$, and we checked that choosing $T = \log^2 N$ was sufficient to eliminate transient effects. Because the number of sites we need to update at each time-step grows like $\log N$, the computer time needed to measure the speed and the diffusion constant for one set of parameters increases as $(\log N)^3$.

To check the accuracy of the measurements, the velocities and diffusion constants obtained from both time intervals ($5T$ and $50T$) are represented using the same symbols on all the plots in this paper. For the velocity, the two symbols are usually so well superposed that only one can be seen. For the diffusion constant, there are few cases where one can see a very small shift, indicating that the diffusion constant D_N is more difficult to measure than the velocity v_N.

3.2. Diffusion Constant

If $y(t)$ is the position of the front at time t, the definition of D_N we used is

$$D_N = \lim_{t \to \infty} \frac{\langle y(t)^2 \rangle - \langle y(t) \rangle^2}{t} \tag{15}$$

Figure 1 presents the diffusion constant for two values of p on a graph with a logarithmic scale on the vertical axis and a bi-logarithmic scale on the horizontal axis. The symbols are nicely aligned, indicating that the diffusion constant decays like a power-law in $\log N$;
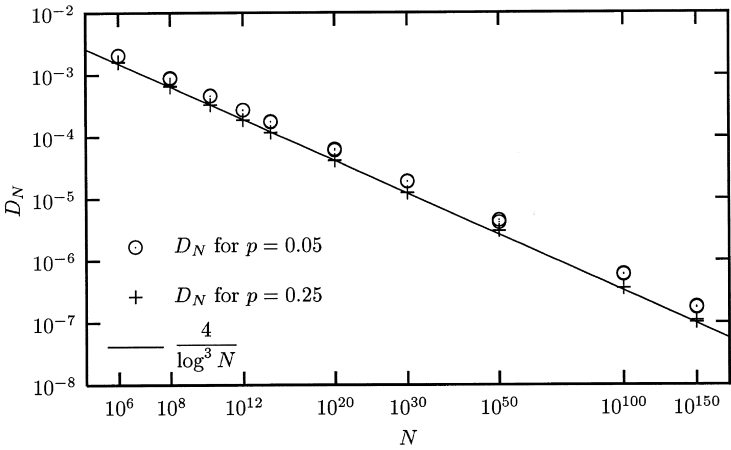
$$D_N \simeq \frac{K'}{\log^\alpha N} \tag{16}$$

Fig. 1. The diffusion constant D_N of the stochastic model described in Section 2. The symbols correspond to two sets of simulations for $p = 0.05$ and $p = 0.25$, and the straight line represents a decay in $4/\log^3 N$. The scale on the horizontal axis is in $\log(\log N)$.

The results are consistent with $\alpha = 3$, but we cannot exclude numerically other values for α. (For instance, $\alpha = 2.9$ fits also quite nicely.) So even with $N = 10^{150}$, we cannot achieve an accuracy better than 0.1 on the exponent α.

3.3. Correction to the Velocity

On Figs. 2 and 3 we have compared the actual velocity correction $v_{\min} - v_N$ to the prediction (13, 14) of the cut-off approximation developed in ref. 29. The $K/\log^2 N$ decay is nicely confirmed and, for very large N, the data seem to agree with the value of K given by (14). Indeed, we have plotted the difference $K_{\text{approx}}/\log^2 N - (v_{\min} - v_N)$ on the same figure, and we see that this second-order correction decays faster (but not *much* faster) than $1/\log^2 N$.

Our data are therefore consistent with a correction to the velocity equal to

$$v_{\min} - v_N = \frac{K_{\text{approx}}}{\log^2 N} + O\left(\frac{1}{\log^\beta N}\right) \tag{17}$$

where K_{approx} is given by (14) and where β is between 2.5 and 3. In any case, as observed in refs. 29, 31, and 33, the second term in the right hand side of (17) is not much smaller (about 15% only) than the first one for values of N of order 10^{15}.
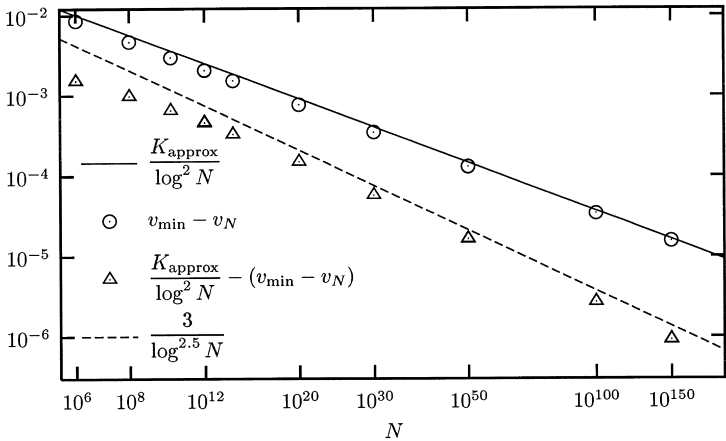
Fig. 2. For $p = 0.25$, correction to the velocity in our stochastic model of Section 2 compared to the prediction of the cut-off approximation of ref. 29 (plain line). The difference $K_{approx}/\log^2 N - (v_{min} - v_N)$ seems to decay faster than $1/\log^2 N$. The dashed line represents a decay in $1/\log^{2.5} N$ as a visual guide.

4. A SIMPLIFIED MODEL

For Fisher-KPP like equations, the velocity is determined by the tail of the front. It is therefore reasonable to think that the main influence of the noise is concentrated at the tip of the front, namely at the sites where the occupation numbers are limited to a few particles. To test this idea, we consider in this section an extremely simplified version of the stochastic model of Section 2.
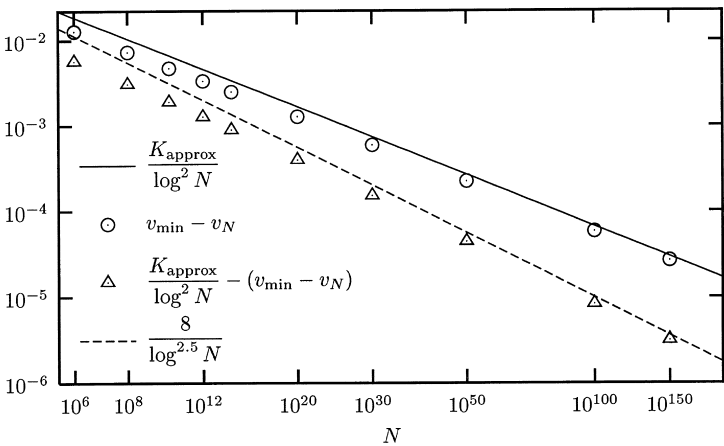

Fig. 3. Same as Fig. 2 for $p = 0.05$.

At each time step, we define the position $x_{\text{tip}}(t)$ of the tip of the front as the smallest x such that $h(x, t) = 0$. Therefore, $x_{\text{tip}}(t)$ is defined by

$$
\begin{aligned}
h(x_{\text{tip}}(t), t) &= 0, \\
h(x_{\text{tip}}(t) - 1, t) &> 0
\end{aligned}
\tag{18}
$$

Then, in this simplified model, $h(x, t)$ evolves in the following way: for all $x < x_{\text{tip}}(t)$, we calculate $h(x, t+1)$ using the deterministic equation (9). Only for $x = x_{\text{tip}}(t)$, we keep the stochastic rule of the model as defined in Section 2, except that we take a Poisson distribution instead of a binomial distribution. (Considering that N is very large and that $h(x_{\text{tip}}(t), t+1)$ is of order $1/N$, the binomial distribution reduces to the Poisson distribution.) In other words, we take

$$
h(x_{\text{tip}}(t), t+1) = \frac{m}{N}
\tag{19}
$$

where the number m of particles at the tip site is chosen according to a Poisson distribution

$$
\text{Proba}(m) = \frac{\langle m \rangle^m}{m!} e^{-\langle m \rangle}
\tag{20}
$$

and where the average occupancy $\langle m \rangle$ is obtained from (8) by

$$
\begin{aligned}
\langle m \rangle &= N \langle h(x_{\text{tip}}(t), t+1) \mid \{h(x, t)\} \rangle \\
&= Np[2h(x_{\text{tip}}(t) - 1, t) - h(x_{\text{tip}}(t) - 1, t)^2]
\end{aligned}
\tag{21}
$$

In this simplified model, the evolution of the front is deterministic everywhere except for a single site at the tip of the front. As a consequence $h(x, t)$ is only quantized for $x = x_{\text{tip}}$ and it takes continuous real values for all $x < x_{\text{tip}}$.

In this simplified model, there is a cut-off of order $1/N$ and we expect that the shift of the velocity decays as $1/\log^2 N$. As there is some randomness at the tip of the front, we also expect a diffusive behavior. To our surprise, we find that both v_N and D_N coincide, for large enough N, with what was obtained in the full model of Sections 2 and 3: As can be seen on Figs. 4 and 5, not only this simplified model has a diffusion constant which seems to decay as $1/\log^3 N$, but *we cannot distinguish for large N the data from the simplified model from those of the original one.* This is also true for
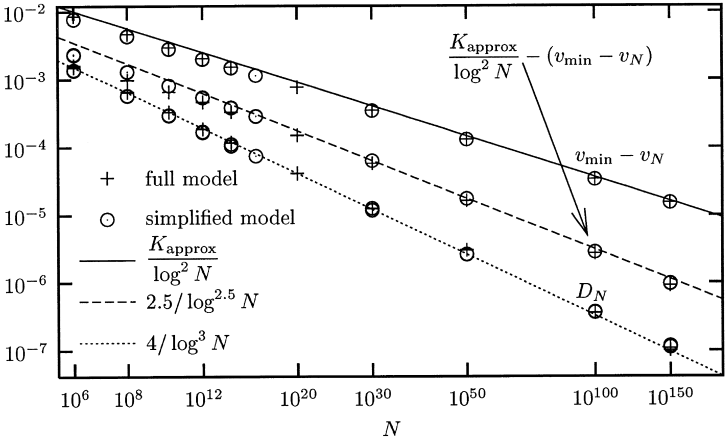
Fig. 4. For $p = 0.25$, a comparaison of different quantities in the full stochastic model of Section 2 and in the simplified model of Section 4. From top to bottom: the velocity correction $v_{min} - v_N$, the difference $K_{approx}/\log^2 N - (v_{min} - v_N)$ and the diffusion constant. The plain line represents $K_{approx}/\log^2 N$ and the two dashed lines decay respectively like $2.5/\log^{2.5} N$ and $4/\log^3 N$.

the second order correction to the velocity (the difference between the prediction (13, 14) given by the cut-off approximation and the actual value of $v_{min} - v_N$). It seems therefore that this simplified model with the noise limited to a single site at the tip of the front captures the large N dependence of v_N and D_N of the full model.
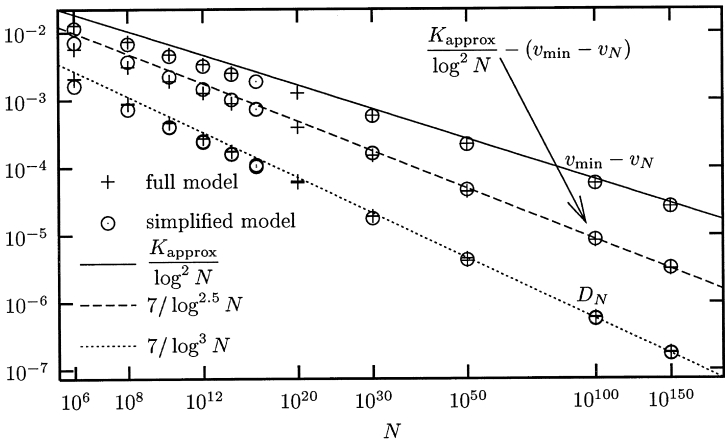

Fig. 5. Same as Fig. 4 for $p = 0.05$.

5. CONCLUSION

In this paper, we have studied numerically the velocity v_N and the diffusion constant D_N of a microscopic system involving N particles, which reduces in the limit $N \to \infty$ to a deterministic Fisher-like equation (9). Our simulations of this model for N up to $N = 10^{150}$ give additional evidence that, for large N, the velocity of such a front is given by the linear marginal stability velocity $v_{\min}$ minus a logarithmic correction in $K/\log^2 N$ (Eq. (3)). Furthermore, our results indicate that the value of the constant K is very close and might possibly be equal to the analytical expression K_{approx} obtained in our previous work[29] for the case of a deterministic front with a cut-off $1/N$.

A second result concerns the diffusion constant D_N of the front. Our data indicate that $D_N \simeq K'/\log^\alpha N$, with $\alpha = 3 \pm 0.1$. A previous attempt[24] to measure a diffusion constant in a similar situation gave a $N^{-0.32}$ decay of D_N for an effective N up to 10^6. We believe that the asymptotic behavior was not yet reached. In fact, a similar apparent power law can be observed for the shift of velocity when N is moderately large,[21] although this shift becomes logarithmic for larger values of N. It would, of course, be interesting to confirm this logarithmic decay of D_N for other models which exhibit already the logarithmic shift of the velocity.[30, 32, 33]

Our third and last result concerns a very simplified model (Section 4) where noise is only present at the tip of the front. To our surprise, the shift of velocity $v_{\min} - v_N$ and the diffusion constant D_N seem to be the same for large N as in the full model of Section 2. Therefore, our next efforts to understand analytically (16) and (17) will first focus on this simplified model.

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