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# Dynamic scaling and self-organized criticality in diffusion fronts growth

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**Abstract.** We study the dynamics of the growth process of fluctuating diffusion fronts of interacting particles. The description of the kinetics is based on the mean field master equation within the framework of a lattice gas model. We analyse the time evolution of diffusion fronts by a dynamic scaling approach, and find that the scaling behaviour of these interfaces is characterised by anomalously large exponents which agree with the numerical and experimental results. Using a theoretical model of diffusion fronts' fluctuations developed in [1], we have also illustrated the diffusion fronts' propagation *via* avalanches.

**PACS.** 05.50.+q Lattice theory and statistics (Ising, Potts, etc.) – 05.60.-k Transport processes – 68.35.Fx Diffusion; interface formation

## 1 Introduction

Recently, an enormous amount of work [2–9] has been devoted to the study of the dynamics of growing rough surfaces which may originate from many processes. Some surfaces are formed as a result of a deposition process, others are generated due to erosion or etching and some interfaces are formed spontaneously in inhomogeneous media. In general, these systems are related to out of equilibrium phenomena for which no systematic formalism exists. To this end, a variety of discrete models and continuous equations have been developed with the goal of understanding the generic properties of these diverse growth processes, and to identify the universality classes to which the growth models belong. The simplest model exhibiting kinetic roughening is the Edwards-Wilkinson linear model [10] based on a Langevin-type equation. The first extension of the Edwards-Wilkinson equation to include non-linear terms was proposed by Kardar-Parisi and Zhang, and this gives rise to the KPZ relation [11]. The two-dimensional KPZ model successfully describes a remarkable diversity of growth processes and is an excellent example of universality.

One of the most important quantities used to characterise the scaling of the interfaces is the width $\sigma(L,t)$ which is defined by,

$$\sigma(L,t) = \left(\langle h^2\rangle - \langle h\rangle^2\right)^{1/2}$$

where the function $h(x,t)$ gives the height of the interface at time $t$ and position $x$. $L$ is the system size and $\langle\ \rangle$ denotes a spatial average over the whole system.

For early times, the width is expected to grow as some power of time [12],

$$\sigma(L,t) \sim t^{\beta}$$

the exponent $\beta$ describes the growth of correlation with time along the growth direction. At a characteristic saturation time $t_{\rm c}(L) \sim L^z$ ($z$ is the dynamic exponent), the correlation length reaches the system size leading to the width saturation with a power law dependence on $L$ [12],

$$\sigma(L, t \to \infty) \sim L^{\alpha}$$

where $\alpha$ is the roughness exponent that characterises the surface morphology. Hence, the width $\sigma(L,t)$ satisfies the Family-Vicsek ansatz [12],

$$\sigma(L,t) = L^{\alpha} f(t/L^z)$$

where the scaling function $f(x)$ behaves as,

$$f(x) \sim \begin{cases} x^{\beta} & \text{if} \quad x \ll 1 \\ \text{const} & \text{if} \quad x \gg 1. \end{cases}$$

The fact that a growing surface spontaneously evolves into a steady state with fractal properties, Bak *et al.* [13] have proposed that the dynamics of these systems can be described by a mechanism they call self-organized criticality.

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The latter is supposed to be a natural evolution of extended dissipative systems for which the$1/f^{\gamma}$ noise represents the intrinsic evolution of spatial structure with scale invariant properties. The basic ideas of self-organisation processes are illustrated in the avalanche models introduced by Bak, Tang and Wiesenfeld [13].

In this paper we investigate the motion of nonequilibrium unidimensionel interfaces called diffusion fronts. The latter propagate through an inhomogeneous system of which the static properties are represented by the problem of percolation in a gradient. We have simulated the growth dynamics of diffusion fronts of hard core particles without interaction in a preceding work [14]. Here, we process the case of repulsively interacting particles in which an order-disorder transition occurs, so as to extract the ordering effects on the diffusion fronts. The numerical simulations are performed using the mean field master equation in the context of a lattice gas model and the results are analysed by the dynamic scaling approach. In the second part of this work, we study the dynamics of diffusion fronts in the framework of a self-organized criticality mechanism.

## 2 Mean field lattice gas model

A lattice gas consists of a discretisation of continuous space. The latter is subdivided into cells represented by sites forming a lattice. The sites can be occupied or empty. For each site $i$, we define an occupation number $n_i$ which takes the value 0 or 1 to designate respectively an empty or full site. The set of all the occupation numbers at a given moment is called a configuration. For a lattice of $N$ sites labelled by their coordinates $i = 1, 2, ..., N$; the configuration of particles can be written

$$\{n\} = \{n_1, n_2, ..., n_N\}.$$

When the particles interact, their Hamiltonian is given by

$$H = -\sum_{i>j} \varepsilon_{ij} n_i n_j - \mu_0 \sum_i n_i. \tag{1}$$

For a repulsive interaction, $\varepsilon_{ij} = \varepsilon < 0$ and $\{i, j\}$ are nearest neighbour sites; $\mu_0$ is the bare chemical potential.

To define the dynamics we suppose that the particles can jump to nearest-neighbouring empty sites. This corresponds to the change of the occupation numbers of the lattice sites. Such a dynamic can be treated by the general master equation for the kinetic evolution of the average concentration $p_k = \langle n_k \rangle$ [15]

$$\frac{\partial p_k}{\partial t} = \frac{\partial}{\partial t}\langle n_k \rangle = -\sum_j \langle J_{kj} \rangle \tag{2}$$

$J_{kj}$ is a current operator along the link $k \leftrightarrow j$, which takes the following form

$$J_{kj}(\{n\}) \equiv \omega_{kj}(\{n\}) n_k (1 - n_j) - \omega_{jk}(\{n\}) n_j (1 - n_k) \tag{3}$$

where $\omega_{kj}(\{n\})$ is the jump probability from site $k$ to site $j$ depending on the local configuration. The product $n_j(1 - n_k)$ imposes that the site $j$ is filled while the site $k$ is empty (the hard core exclusion principle).

The model is a hopping model in which the jumps are between nearest neighbour sites. The barrier that the particles have to overcome before making a jump only depends on the depth of the initial site: the saddle point energy is insensitive to the environment and the energy of the final site has no influence on the jump probability. As the thermal energy is supposed small compared to the barrier heights, the jump probability follows an Arrhenius law. This leads to

$$\omega_{kj}(\{n\}) = \omega_0 \exp\left(\frac{-\varepsilon}{K_{\mathrm{B}}T} \sum_{a \neq j-k} n_{k+a}\right) \tag{4}$$

$\omega_0$ is the isolated jump probability, $a$ denotes a lattice unit vector and summation over $a$ means summation over all nearest neighbours.

The kinetic equation (2) is untractable in its present form and simplifications are necessary. The simplest approach is the mean field approximation that consists of replacing all the operators $n_k$ for the jump probabilities $\omega_{jk}$ by their average concentrations $p_k$ at the same site $k$ [16]. The general expression for the current in equation (2) can then be written as

$$\langle J_{kj}(\{n\}) \rangle \equiv \langle \omega_{kj}(\{n\}) \rangle p_k (1 - p_j) - \langle \omega_{jk}(\{n\}) \rangle p_j (1 - p_k) \tag{5}$$

where

$$\langle \omega_{kj}(\{n\}) \rangle = \omega_0 \exp\left(\frac{-\varepsilon}{K_{\mathrm{B}}T} \sum_{a \neq j-k} p_{k+a}\right). \tag{6}$$

For systems of particles with repulsive interaction, an order-disorder transition arises at a critical temperature $T_{\mathrm{c}}$. As a consequence, a symmetry breaking is present at low temperature. It is then convenient to distinguish the various sublattices by different "colors". In the case of a square lattice, the ordered phase consists of an ordering onto a checkerboard lattice formed with two sublattices with colors A and B. On each sublattice, a concentration can be defined and it is supposed by hypothesis to vary slowly in space: $p_k^{\mathrm{A}}$ and $p_k^{\mathrm{B}}$ are then defined for $k$ belonging as well to A or B. Equation (2) then becomes

$$\frac{\partial p_k^{\mathrm{A}}}{\partial t} = -\sum_{j=k+a} \langle J_{kj}^{\mathrm{AB}}(\{n\}) \rangle \tag{7a}$$

$$\frac{\partial p_j^{\mathrm{B}}}{\partial t} = -\sum_{k=j+a} \langle J_{jk}^{\mathrm{BA}}(\{n\}) \rangle \tag{7b}$$

where

$$J_{kj}^{\mathrm{AB}} \equiv \langle \omega_{kj}^{\mathrm{AB}} \rangle p_k^{\mathrm{A}} (1 - p_j^{\mathrm{B}}) - \langle \omega_{jk}^{\mathrm{BA}} \rangle p_j^{\mathrm{B}} (1 - p_k^{\mathrm{A}}). \tag{8}$$

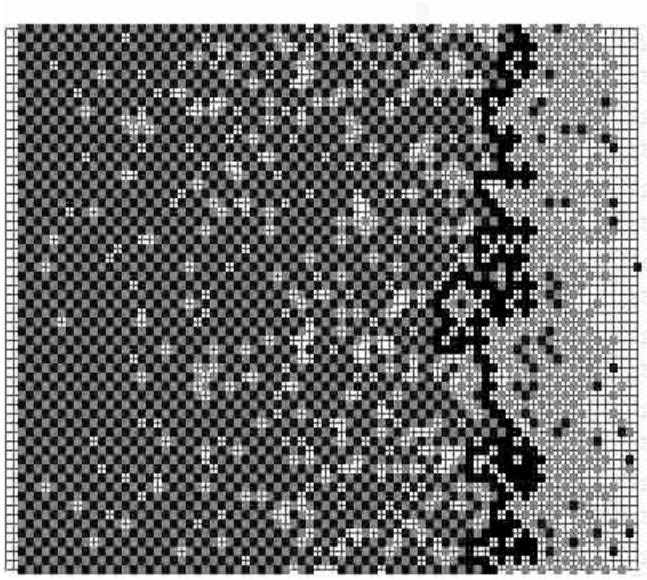

**Fig. 1.** The distribution of the concentration profile, solution of equations (7), on a square lattice. The black and grey sites indicate different sublattices. The bold line illustrates the diffusion front.

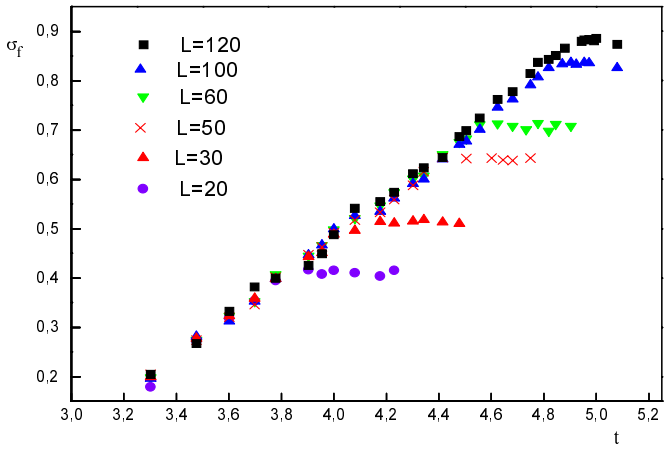


**Fig. 2.** Log-log plot of the diffusion front width *versus* time for different system sizes ($L$). The best fit of the linear region (before saturation) gives the slope $\beta = 0.41 \pm 0.01$.

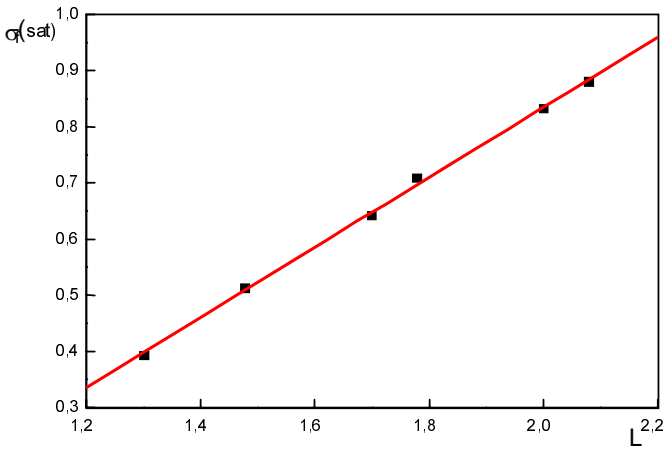


**Fig. 3.** A plot of the saturated interface width as a function of the samples size on log-log plot. The continuous line fits the data and gives the roughness exponent $\alpha = 0.62 \pm 0.01$.

## 3 Dynamic scaling of diffusion front growth

The calculations are restricted to the repulsive interactions in the low temperature regime and are performed using a set of particles diffusing in the presence of a concentration gradient on a square lattice of dimensions $L$ and $L'$. The length $L'$ is large compared to the width $L$. The concentration of diffusers $p$ is fixed at one for $x = 0$ and at zero for $x = L'$. The numerical resolution of equations (7) shows that the dynamics of the diffusion process is characterised by an order-disorder transition which consists of the break down of lattice occupation symmetry by filling one sublattice at the expense of the other (one sublattice being empty and the other filled at $p = 0.5$). This order-disorder transition is well discussed in [15]. We distribute the concentration profile solution of (7) on a square lattice by associating to each site of the lattice at random a positive value less than one. The value is then compared to the one of the density profile at the same abscissa. The result of the comparison defines the occupation state of the lattice sites: if the random number is less than the value of the concentration at the same site the latter will be occupied; otherwise the site remains empty. Figure 1 shows the behaviour of diffusing particles under the above conditions. The outermost line of particles still connected to the source is the diffusion front. The latter can be seen also as an interface delimiting disordered region from the ordered one. Our calculation of the front fractal dimension gives a value ($D_f = 1.75 \pm 0.05$) close to that of the diffusion front of noninteracting particles. We analyse the temporal evolution of the diffusion front width by a dynamic scaling approach. Thus, we report the interface width $\sigma_f(L, t)$ ($L$ is the system lateral size) *versus* time $t$ for different sample sizes in Figure 2 on log-log plot. We find that before saturation, $\sigma_f$ increases with the exponent $\beta = 0.40 \pm 0.01 (\sigma_f \sim t^\beta)$. The front saturated width sketched as a function of the system lateral size in Figure 3 on a log-log plot leads to a roughness exponent $\alpha = 0.62 \pm 0.01$ in $\sigma_f(\text{sat}) \sim L^\alpha$. We have observed in our simulations that the front localisation depends on the interaction regime recovering, thus the results of references [17,18] where it was displayed that the diffusion front of interacting systems can be assimilated to the hull of interacting percolation problem for which the percolation threshold depends on the interaction regime ($p(x_f, \gamma, t \to \infty) = p_c(\gamma)$).

As mentioned above, we have undertaken the same calculations in the case of the front of noninteracting diffusing particles in a previous work [14] and we have found that the front grows with an exponent $\beta = 0.40 \pm 0.01$ and saturates with an exponent $\alpha = 0.62 \pm 0.01$. Hence,

the order-disorder transition does not influence the scaling behaviour of diffusion fronts; only its localisation is affected by the interactions.

## Discussion

The scaling exponents obtained for an interacting system coincide with those of the noninteracting case (taking into account the interval error) as indicated above. This result is consistent with the universality concept. These scaling exponents' values belong to the scaling picture developed by different experiments and simulations concerning driven interfaces moving in disordered media (fluid flow in porous media, paper wetting) [19–24]. This can be explained by the fact that the diffusion fronts and the invasion fronts exhibit the same fluctuations behaviour [25]. Indeed, taking inspiration from previous results [1,25], we assume that our model is appropriate to the problem of injection of a fluid in a porous media in the bidimensional case: the finite ordering clusters of particles correspond to the pores clusters in the fluid-flow experiments, the concentration plays the role of fluid pressure and the noise generated by the fluctuations of a front's length is identified with the noise of fluid pressure fluctuations in the invasion experiments. The diffusion front is an interface propagating in a disordered medium, in which the driving force can be expressed as: $F \sim 1/|\nabla p|$ (where $\nabla p$ is the local concentration gradient) and is located at a critical concentration $p_c$ corresponding to a critical driving force $F_c \sim 1/|\nabla p_c|$ ($|\nabla p_c|$ denotes the concentration gradient at $p_c$). Although the particles are mobile in our model, there exist at any time $t$ finite ordered clusters in the vicinity of the diffusion front. Hence, the motion of the latter is done through frontiers delimiting the clusters. Taking into account the stationary behaviour of the diffusion front for infinite times, we can assume that the random distribution of ordered clusters just nearby the front is static and in average it has the same effect as the quenched disorder. This is confirmed by the obtained scaling exponents being larger than those predicted by the EW and the KPZ universality in $(1+1)$ dimensions as it is known that quenched disorder generates anomalously large exponent values. Thus, the diffusion fronts possess the same features as the interfaces that move in the presence of quenched noise.

## 4 Self-organized criticality in diffusion front growth

### 4.1 The front fluctuations model

Particular attention was given to the fluctuations of the diffusion front as it makes easier studies of interface instabilities. Numerical calculations [1] had provided

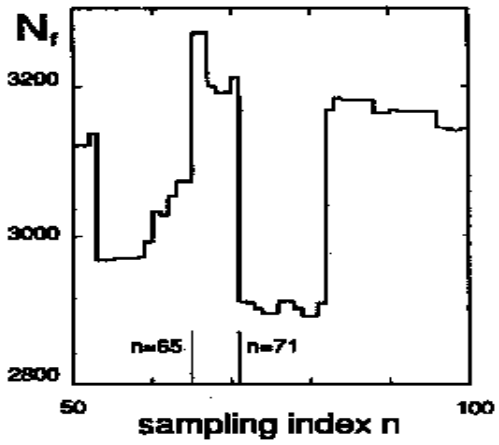


**Fig. 4.** Time evolution of the number $N_f$ of particles on the diffusion front (from Ref. [1]).

a so-called "catastrophic events" rising through connection/disconnection process of clusters of large size by the jump of a single particle. As shown in Figure 4, a microscopic process may induce remarkable changes of the number of particles on the front in a time scale of the order of one particle hopping time. The simulations have been performed considering only hard core interaction and it was found that fluctuations of the length of the front behave like a power law with the Hurst exponent,

$$\left\langle \Delta N_f(t)^2 \right\rangle = \left\langle \Big( N_f(t) - N_f(0) \Big)^2 \right\rangle \sim t^{2H}. \qquad (9)$$

There exists a crossover time $t^*$ which delimits two regimes. The first regime ($H = 1/2$) corresponds to time intervals shorter than $t^*$ where fluctuations are linear with time ($1/f^2$ noise). For the second regime ($H = 0$), the fluctuations saturate ($1/f$ noise).

Gouyet and Boughaleb have developed a theoretical model to describe the connection/disconnection process of front fluctuations [1]. The model is based on knowledge of clusters distribution in vicinity of the front and probability of appearance of fluctuation of size $h$. Some little changes in defining the diffusion front are included to allow better characterisation of the fluctuations. The front is assimilated to a seashore which delimits islands from lakes. Thus, the fluctuations of the front are determined by connection/disconnection of islands (particle clusters) or by closure/opening of lakes (clusters of empty sites) by jump of an only one particle. To simplify the presentation, taking into account the similarity of the scaling laws, only the connection/disconnection process of clusters is considered and there is no correlation between two successive fluctuations of the front length . Let $M_h(p)$ be the number of clusters with $h$ sites on their hulls. These clusters are centred in a region of concentration $p$ and are able to be connected or disconnected by only one particle jump. In this region, $m_h(p)$ of $M_h(p)$ are

supposed to be connected at a given time. The probability of the connection/disconnection process is governed by the Smolochowski equation which can be written as [1],

$$\frac{\partial P(m_h,t)}{\partial t} = 2\Pi_h P(m_h,t) - (2m_h - M_h)\Pi_h \frac{\partial P(m_h,t)}{\partial m_h} + \frac{M_h \Pi_h}{2}\frac{\partial^2 P(m_h,t)}{\partial m_h^2} \quad (10)$$

where $\Pi_h$ denotes the elementary probability of connecting/disconnecting one particular cluster among the $M_h(p)$ and is related to "$\tau_r = 1/2\Pi_h(p)$" the characteristic relaxation time of the system in a region of concentration $p$.

The development of calculations using equation (10) allows to recover analytically the expression of front length fluctuations shown numerically by relation (9) and to determine the density of events $N_{ev}(h)$ that is the number of events of size $h$ per time unit (connection or disconnection of a cluster of size $h$). The density of events of size $h$ is of great interest as it permits us to link with the avalanche models for self-organized criticality. It has been displayed that it takes the following form [1],

$$N_{ev}(h) \sim h^{-y_h} \quad (11)$$

where $$y_h = 2 - \frac{1}{\upsilon D_f} = 1.5714...$$

Equation (11) has been confirmed numerically in [26].

### 4.2 Analogy between the diffusion front fluctuations model and the avalanche models

Following the evolution of the diffusion front, we notice that the catastrophic events happen once the front goes away from the percolation threshold $p_c$ due to connection or disconnection of clusters (frequent small events in Fig. 4) just nearby it. This can be explained by the fact that each time the diffusion front deviates from $p_c$, it evolves spontaneously (without the intervention of an adjusting force) in order to restore its critical state corresponding to a fractal structure centred in the region of concentration $p_c$. In other words, the fluctuations rule self-tunes the diffusion front such that it is always at the critical point $p_c$ by connection or disconnection of large clusters characterised by a power law density $N_{ev}(h)$. The temporal signature of such an evolution as shown in the previous section is the flicker noise. Thus, one can easily deduce that the front fluctuation is a self-organized critical phenomenon of which the general mechanism is similar to the avalanches process. Indeed in models of avalanche, the condition that insures the criticality is, in general, linked to the average height $\theta$. If $\theta$ exceeds a critical value $\theta_c$, due to the addition of grains; one assists therefore to the avalanches. The particles provided by the source in our model induce the diffusion leading to the connection/disconnection process of clusters neighbouring the front which causes the deviation of the front from its critical state. These particles perturb the system playing then the role of the external flow of grains in the avalanche models. The avalanches arise to restore the critical state of the pile like the large fluctuations (catastrophic events) in the front model and the two processes are distributed as a power law of same form. Thus, it is clear that the critical concentration $p_c$ denotes the critical height $\theta_c$ in the avalanche models language, the particles provided by the source in the front model are identified to the added grains in the avalanche models and the large fluctuations represent the avalanches. All arguments above display that the diffusion front is an extended dissipative system as it keeps its fractal geometry and presents a $1/f$ noise; it evolves according to a self-organized critical mechanism which can be described by the avalanches process.

## 5 Conclusion

In summary, we have displayed that the order-disorder transition influences only the localisation of the diffusion front. The front width $\sigma_f(L,t)$ satisfies the dynamic scaling Family-Vicsek ansatz [12] ($\sigma_f(L,t) = L^\alpha f(t/L^z)$) with critical exponents $\alpha$ and $\beta$ which are anomalous in the sense that they are larger than the EW and the KPZ exponents. Given the similarity between the diffusion and the invasion fronts fluctuations, we have explained this anomalous roughening by the presence of finite ordering clusters in vicinity of diffusion front. This constitutes an inhomogeneous disorder that has the same effect as the quenched randomness generated by the pores in the fluid-flow experiments. We have also shown that the diffusion front propagation is a self-organized critical phenomena by establishing an analogy between the front fluctuations model and the avalanche models.

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