Dynamics of diffusive rough interfaces in inhomogeneous systems

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We investigate the dynamics of interfaces growth in inhomogeneous systems. The description of the kinetics is based on the mean field master equation in terms of lattice gas model. The existence of repulsive interactions between nearest-neighbour particles creates an order in the system. We show that the order extension has an influence on the localisation of the diffusive interface called "the diffusion front" which delimits disordered region from ordered one. We analyze the time evolution of diffusion fronts by dynamic scaling approach and we find that the scaling behavior of these interfaces is characterized by anomalously large exponents which agree with the experimental and theoretical results.

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I. INTRODUCTION

In the last few years, a great interest has been focused in understanding the dynamics of rough interfaces which can be found in various physical situations (crystal growth, magnetic domain, thin films corrosion, directed polymers in random media..)where some surfaces are formed as a result of a deposition process, others are generated due to erosion or etching and some interfaces propagate through inhomogeneous media. In general, these systems are related to out of equilibrium phenomena for which no systematic formalism can treat. To this end, several computer models and theoretical approaches have been developed [1, 2, 3] with the goal of understanding the generic properties of different growth processes. One of the modern concepts used to study various roughening processes is the dynamic scaling approach: the surface width σ obeys the scaling form : $\sigma(L, t) = L^{\alpha} f(t / L^{z})$ where f is a scaling function hence defined: $f(x) \sim x^{\beta}$ for $x<<1$ and $f(x) \sim constant$ for $x>>1$ with $z=\alpha/\beta$ representing the dynamic exponent; α and β are exponents characterizing how the surface width grows with the length scale L and the time t. The Edwards-Wilkinson equation [4], based on Langevin type equation, was the first continuum equation used to study the growth of interfaces by particles deposition. The predictions of this linear theory change, however, when non linear terms are added to the growth equation. The first extension of the Edwards-Wilkinson equation to include non linear terms was proposed by Kardar ,Parisi and Zhang [5]. The K P Z equation is capable of explaining not only the origin of the above scaling form but it gives also the exact values of the scaling exponents for one dimensional interfaces ($\alpha= 1/2$; $\beta = 1/3$) and provides a relation between two unknown exponents α and z in any dimension ($\alpha + z = 2$). A variety of models [6] argue that the values of α and β are in agreement with the analytical results of K P Z. However, more recently it has been shown that in experiments on two fluid flow in porous media [7, 8] and in a number of models [9-12], the exponents are anomalous and do not agree with the K P Z result.

Up to now, most of the studies have concerned only the dynamics of the growth and the formation of rough interfaces. In this paper, we will be discussing, in addition, the ordering finite size effect on these interfaces. For this purpose, we treat first the dynamics of the diffusion front by dynamic scaling approach for a system of hard core particles without interaction. Then, we consider a system of repulsively interacting particles submersed in a regular potential crystalline and constraint to diffuse under a concentration gradient. The calculations are performed using the mean field approximation in the context of lattice gas model. The dynamics of the interface growth is analyzed by dynamic scaling approach .

II. THE LATTICE GAS MODEL

A. The Model

The model is presented in some detail in [15]. Here, we only give a brief summary. We consider a square lattice of N sites; each site can be occupied or empty and n_i={0, 1} denotes occupation (n_i=1) or nonoccupation (n_i=0) of site i. Let the configuration {n} be the set of occupation numbers for each site that we note for a lattice with N sites as,

$$\{n\}=\{n_1, n_2, ...,n_N\} \quad (1)$$

The Hamiltonian for a given configuration *{**n**} is given by,*

$$H = -\sum_{i>j} \varepsilon_{ij} n_i n_j - \mu_o \sum_i n_i \quad (2)$$

where μ_o is the bare chemical potential and ε_{ij} is the interaction energy between the sites i and j.

The diffusion process of the particles is insured by the change of the occupation numbers of the lattice sites. In the lattice gas formulation, this can be seen as the change of the lattice configuration. The dynamics of the lattice is then

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governed by the phenomenological master equation which describes the evolution in time of the probability $P(\{n\}, t)$ of having the configuration $\{n\}$ at time t,

$$\frac{\partial P(\{n\},t)}{\partial t} = \sum_{\{n'\}} \omega(\{n'\},\{n\})P(\{n'\},t) - \omega(\{n\},\{n'\})P(\{n\},t) \quad (3)$$

The rate of the configurations exchange is expressed by the transition frequency $\omega(\{n\}, \{n'\})$ which encodes all physical information about the system considered.
The average concentration over all possible configurations is defined by,

$$p_k = \langle n_k \rangle = \sum_{\{n\}} n_k P(\{n\},t) \quad (4)$$

The kinetic evolution of the average concentration $p_k = \langle n_k \rangle$ at site k, is governed by the general master equation,

$$\frac{\partial p_k}{\partial t} \equiv \frac{\partial}{\partial t}\langle n_k \rangle = \sum_j \left\langle \omega_{jk}(\{n\}) n_j (1-n_k) - \omega_{kj}(\{n\}) n_k (1-n_j) \right\rangle \quad (5)$$

where $\omega_{jk}(\{n\})$ is the jump probability from site j to site k, 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). We restrict the jumps to those between nearest neighbor sites k and $k+a$. Hence, it is convenient to introduce a current operator $J_{k,k+a}(\{\boldsymbol{n}\})$ along the bond $k \rightarrow k+a$. Equation (5) becomes then ,

$$\frac{\partial p_k}{\partial t} = -\sum_a \left\langle J_{k,k+a}(\{\boldsymbol{n}\}) \right\rangle \quad (6)$$

(where we have taken $j=k+a$ in equation (5)).

The average current in the bond (i,j) is,

$$\left\langle J_{ij}(\{n\}) \right\rangle \equiv \left\langle \omega_{ij}(\{n\}) n_i (1-n_j) - \omega_{ji}(\{n\}) n_j (1-n_i) \right\rangle \quad (7)$$

For systems of particles with repulsive interactions, an order - disorder transition rises at a critical temperature T_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 in 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 : ${p^A}_k$ and ${p^B}_k$ are then defined for k belonging as well to A or B. Equation (6) then becomes,

$$\frac{\partial p_i^A}{\partial t} = -\sum_{j=i+a} \left\langle J_{ij}^{AB}(\{n\}) \right\rangle \quad (8a)$$

$$\frac{\partial p_j^B}{\partial t} = -\sum_{i=j+a} \left\langle J_{ji}^{BA}(\{n\}) \right\rangle \quad (8b)$$

where

$$J_{ij}^{AB} \equiv \omega_{ij}^{AB} n_i^A \left(1-n_j^B\right) - \omega_{ji}^{BA} n_j^B \left(1-n_i^A\right) \quad (9)$$

The model is a hopping model in which the jumps are between nearest neighbor 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,

$$\omega_{ij}^{AB}(\{n\}) = \omega_o \, exp\left| -\frac{\varepsilon}{k_B T} \sum_{a \neq j-i} n_{i+a}^B \right| \quad (10)$$

ω_o is the isolated jump probability and ε denotes the interaction energy of the pair nearest neighbor particles. ε is taken negative in order to represent repulsive interaction.

B. Mean field approach

The mean field approximation is the simplest method that allows a primary understanding of the studied phenomenon by providing exact mathematical solutions although it can not describe completely the physical reality. In our case, the consideration of the mean field approach consists in replacing all the occupation numbers n_k by their average concentration p_k [16]. Then, the general expression for the current in equations (8) for the mean field approach can be written,

$$J_{ij}^{AB} \equiv \omega_{ij}^{AB} p_i^A \left(1-p_j^B\right) - \omega_{ji}^{BA} p_j^B \left(1-p_i^A\right) \quad (11)$$

where

$$\omega_{ij}^{AB}(\{n\}) = \omega_o \, exp\left| -\frac{\varepsilon}{k_B T} \sum_{a \neq j-i} p_{i+a}^B \right| \quad (12)$$

III. THE DIFFUSION FRONT BEHAVIOUR FOR THE IDEAL LATTICE GAS

The ideal lattice gas model corresponds to the absence of interaction except the hard core exclusion . The evolution equation of the density profile is simply the second Fick's law which can be deduced from (5) with a zero value of the reduced interaction ($\gamma = -\varepsilon/k_BT = 0$). The diffusion is performed on a square lattice semi-infinite in the x direction ($x>0$) and periodically bounded in the perpendicular direction y. There is a source at the position $x=0$ $(p(x=0, \forall t)=1)$ which feeds the initial empty system and a well at sufficiently large abscissa $(p(x_M, \forall t) = 0)$. Then, the mean concentration solution of the second Fick's law is given for the adopted external conditions by the complementary error function,

$$p(x,t) = erfc(x / l_D) = 1 - (2/\sqrt{\pi}) \int_0^{x/l_D} du\, exp(-u^2) \quad (13)$$

where l_D is the diffusion length ($l_D = 2(Dt)^{1/2}$ where D denotes the diffusion coefficient).

We distribute the density profile solution of (5) on a square lattice by associating to each site of the square lattice at random a positive value less than one. The value is compared to the concentration profile one at the same abscissa obtained by solving the equation (5). 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 noninteracting particles under the above conditions. The outermost line of particles still connected to the source is the diffusion front.

Studies of the diffusion front focus both on its geometrical and dynamical properties. It was shown that the structure of the diffusion front for a system of non interacting particles is fractal and is related to the hull of percolation clusters[17]. Indeed, the diffusion front is located around a concentration region which converges rapidly to p_c [13] the critical percolation threshold for a square lattice. The region of the front in width σ_f around concentration p_c is the region where fluctuations are important. The front length N_f that is the total number of particles in the front, as well as the front width follow power laws as a function of diffusion length. Regarding the diffusion front as the external frontier of the percolation cluster (the hull), the power laws are expressed in term of concentration gradient which is exactly the slope of the density profile around the critical concentration $p(x_f, t, \gamma = 0) = p_c$ and the exponents are related to those of the percolation [13, 14],

$$N_f \sim |\nabla p|^{-\alpha_N} \quad (14)$$

$$\sigma_f \sim |\nabla p|^{-\alpha_\sigma} \quad (15)$$

with $\alpha_N = \alpha_\sigma (D_f - 1)$; $\alpha_\sigma = \upsilon / 1+\upsilon$; D_f is the fractal dimension of the front and υ is the critical exponent associated to the correlation length of percolation $(\xi \sim p-p_c{}^{-\upsilon})$.

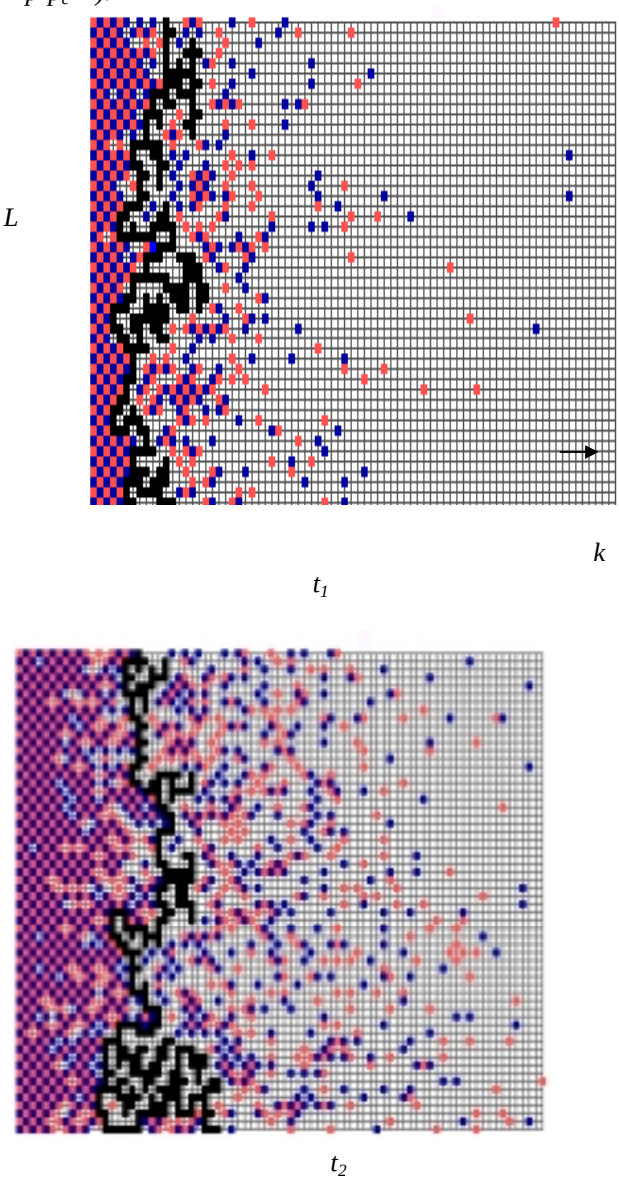

Fig.1 The bold lines represent the diffusion front for the ideal lattice gas. The black and grey sites point out the different sublattices. t_1 and t_2 indicate two different times of particles diffusion ($t_1<t_2$).

Our simulations concern the dynamics growth of the diffusion front width which is defined as the standard deviation of the heights h(k) and is computed from the relation $\sigma_f(L,t) = \sum_{i=1}^{L} \left(h(i) - \bar{h}\right)^2 / L$. We analyse the obtained results by dynamic scaling approach. Thus, we report the interface width $\sigma_f(L, t)$ (L is the system lateral size) versus time t for different samples sizes in fig. 2 on log-log plot. We find that before saturation, σ_f increases with the exponent $\beta = 0.40 \pm 0.01$ ($\sigma_f \sim t^\beta$). The saturated width is sketched as a function of the system lateral size in fig. 3; the slope of the log-log plot leads to an exponent $\alpha = 0.62 \pm 0.01$ in $\sigma_f(sat) \sim L^\alpha$.

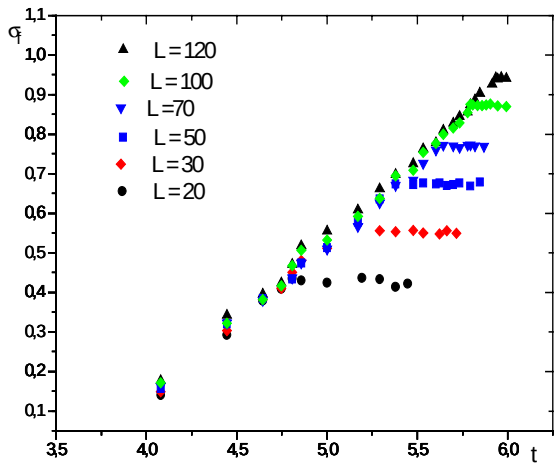

Fig.2 Log-log plot of the diffusion front width versus time for different system sizes (L) in the noninteracting case. The best fit of the linear region gives the slope $\beta = 0.40 \pm 0.01$.

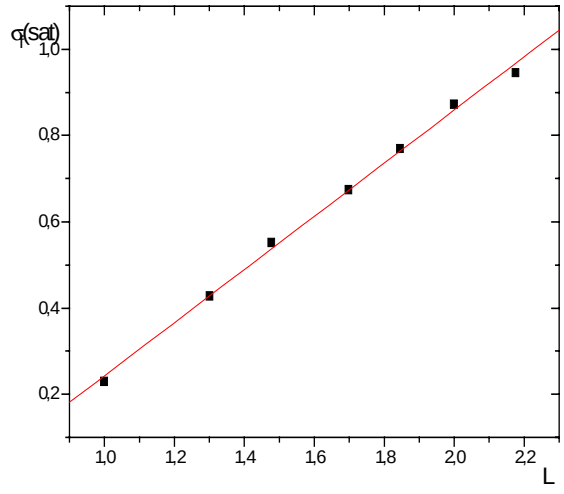

Fig. 3 A plot of the saturated interface width for non interacting system as a function of the samples size on log-log plot. The best fit (continuous line) gives the slope $\alpha = 0.62 \pm 0.01$.

IV. THE DIFFUSION FRONT IN THE INTERACTING CASE

A. The ordering effects on the diffusion front

For interacting lattice gas, the diffusion is performed using the same system as in the non interacting case. Numerical resolution of equations (8) shows that the order-disorder transition arises by the break down of lattice occupation symmetry at a minimal concentration and that the order extension consists in filling one sublattice at the expense of the other (fig. 4). The diffusion front can be seen this time as an interface which delimits disordered region from ordered one (fig.5).

The diffusion front preserves its fractal aspect in presence of the repulsive interactions. Indeed, our calculation of the fractal dimension in this case gives a value close to the the fractal dimension for the ideal lattice gas (D_f =1.7 5± 0.05). The lattice occupation and the order parameter sketched as a function of the mean concentration for different reduced interactions energies in fig. 4, show that the concentration corresponding to the break down of lattice occupation symmetry increases with the reduced interaction energy. This proves that the concentration of the front mean position $p(x_f, t)$ depends on the interaction regime since the diffusion front is the limit between disordered and ordered regions. Thus, the diffusion front is identified to the hull of interacting percolation clusters .This behaviour is confirmed in [13] where it was displayed that the front for interacting diffusion is located at a concentration which tends towards the percolation threshold for homogeneous interacting percolation problem ($p(x_f, t, \gamma) = p_c(\gamma)$ *as* $t \to \infty$). Hence, the concentration corresponding to the front mean position for interacting systems allows to estimate the percolation threshold very accurately.

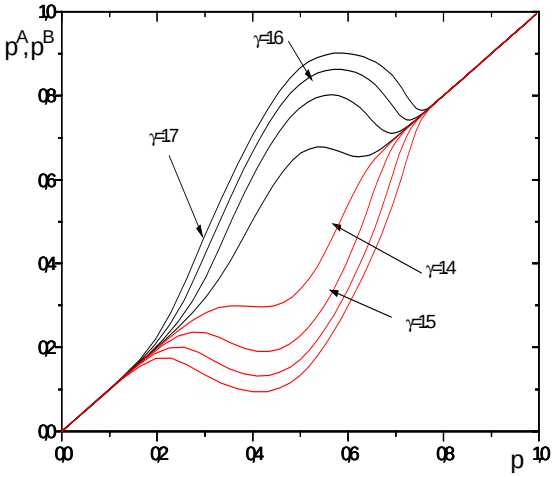

Fig. 4a The break down of the occupation symmetry of the square lattice for different reduced energies and the sublattices occupation.

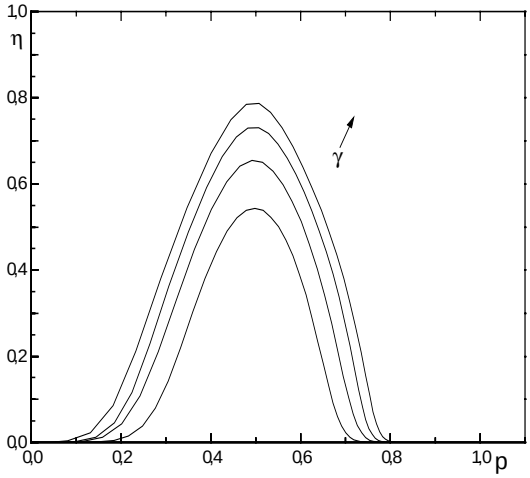

Fig. 4b The order parameter η defined as the difference between the occupation of the two sublattices A and B ($\eta(k)=p_k^A-p_k^B$)versus concentration for different reduced energies.

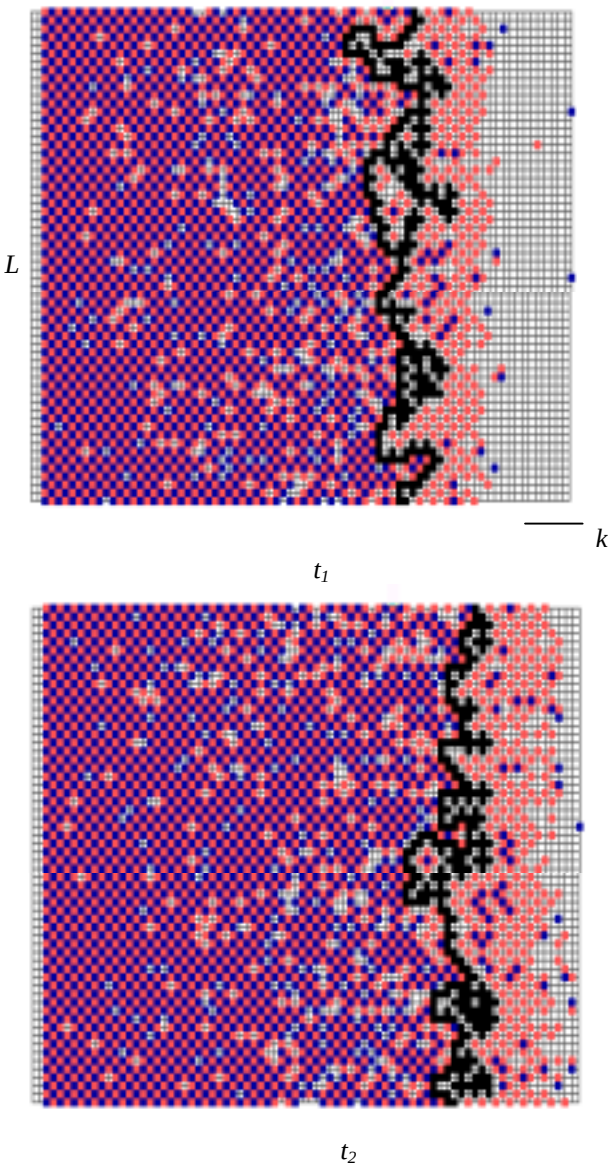

Fig. 5 The diffusion front for a repulsively interacting particles (γ=2) for two different diffusion times (t_2>t_1). Grey and black sites indicate different sublattices. The front appears as a frontier between disordered and ordered regions.

B. Dynamic scaling of the diffusion front growth and discussion

A plot of the time evolution of the diffusion front width in presence of repulsive interactions is shown in fig. 6 on log-log plot. The diffusion front grows with the exponent $\beta = 0.41 \pm 0.01$ and saturates with the exponent $\alpha = 0.62 \pm 0.01$ (fig. 7).

The scaling exponents obtained for a noninteracting system coincide with those of interacting case (taking into account the interval error). This result is consistent with the universality concept. These scaling exponents values belong to the scaling picture developed by different experiments (fluid flow in porous media, paper wetting) [7, 8, 18, 19, 20, 21]]. This can be explained by the fact that the diffusion fronts and the invasion fronts exibit the same fluctuations behavior [22]. Indeed, taking inspiration from previous results [14], we assume that our model is appropriated to the problem of injection of a fluid in a porous media in the bidimensional case : the finite 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 fronts length is identified to 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 ∇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). In the case of fluid-flow experiments, the pores act as a source of quenched randomness which generates larger exponents. We assume that finite clusters in vicinity of diffusion front (the inhomogeneities in our system) have the same effect as the quenched disorder in generating an anomalously large exponents values (the obtained scaling exponents α and β are larger than ($\alpha = 1/2$; $\beta = 1/3$) the KPZ prediction and ($\alpha = 1/2$; $\beta = 1/4$) the Edwards-Wilkinson prediction). Moreover, our estimate of the roughness exponent α ($\alpha = 0.62 \pm 0.01$) is in good agreement with the theoretical value ($\alpha \approx 0.63$) predicted by directed percolation depinning model [1]. Hence, the diffusion fronts possess the scaling properties of interfaces moving in the presence of quenched noise and the inhomogeneous disorder in our model has the same influence on the scaling behavior of diffusion fronts as the quenched noise on the others driven interfaces.

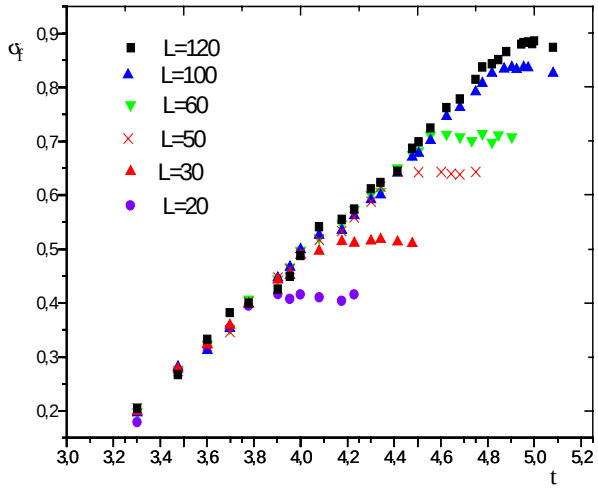

Fig.6 The time evolution of the diffusion front width for different system sizes in the interacting case. The best fit of the linear region (before saturation) gives the slope $\beta = 0.41 \pm 0.01$.

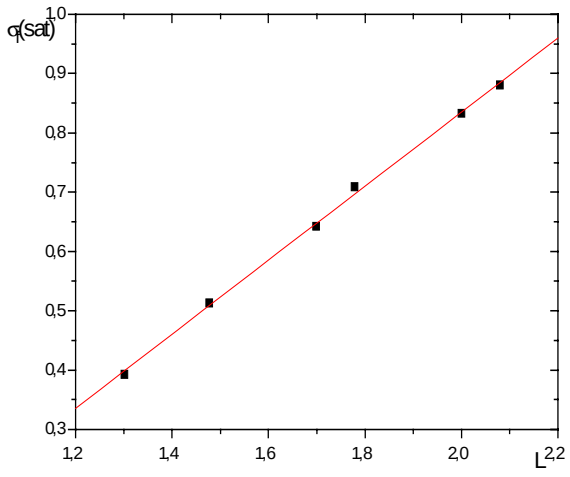

Fig. 7 Saturated width of the diffusion front as a function of the system lateral size on log-log plot. The continuous line fits the data and gives the slope $\alpha = 0.62 \pm 0.01$.

V. CONCLUSION

In summary, we have displayed that the order-disorder transition influences only the localisation of the diffusion front. The latter is similar to the clusters of interacting percolation problem for which the percolation threshold depends on the interaction regime. The diffusion front width $\sigma_f(L, t)$ satisfies the dynamic scaling Family-Vicsek ansatz ($\sigma_f (L, t) = L^{\alpha} f (t / L^{z})$) with critical exponents α and β which are anomalous in the sense that they are larger than the Edwards-Wilkinson and the KPZ exponents. Being based on the similarity between the diffusion fronts fluctuations behavior and those of invasion fronts previously elaborated, we have explained this anomalous roughening by the presence of finite clusters in vicinity of diffusion front. This constitute an inhomogeneous disorder that has the same effect as the quenched randomness genereted by the pores in the fluid-flow experiments.

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