

Scaling behaviour in driven diffusive systems: The example of a bi-dimensional system

R. Nassif^{1,2}, A. Memsouk¹ and Y. Boughaleb^{1,*}

¹*Laboratoire de Physique de la matière Condensée. Université Hassan II-Mohammedia, Faculté des Sciences Ben M'Sik, Casablanca-Maroc*

²*Laboratoire de Physique de la Matière Condensée. Université Chouaib Doukkali, Faculté des Sciences, El jadida-Maroc*

The investigations consider a driven lattice gas of interacting particles with open boundaries within a mean field treatment. We confirm the result obtained by J. Krug that the external conditions induce a phase transition. In the case of a square lattice with repulsive interactions, the phase transition is an order-disorder one which leads to the coexistence of ordered and disordered domains. The dynamical phase transition consists in the break down of the lattice occupation symmetry then in a rapid relaxation of the order parameter. The latter regime is characterised by the growth of the available space for the superstructure till the saturation of the maximal value of the order parameter. The onset of this steady state leads the dynamical phase diagram to approach the statical one except round critical points. A preliminary study of the interface delimiting the ordered and disordered regions is also given. We show that the transition influences the localisation of the interface called: "the diffusion front".

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I. INTRODUCTION

This last decade, driven diffusive systems have been intensively studied but still constitute an intriguing realm of non-equilibrium steady states [1-4]. The example considered here is not directly related to any particular case but can deal with different physical situations where the diffusion process of mobile particles leads to the appearance of a bi-dimensional superstructure at a determined critical temperature [5-7]. Even though the phenomenon is of particular interest, there are only few experimental investigations and the theoretical analysis is quit difficult. In effect, on the one hand such system presents different phase transitions giving rise to multiple bi-dimensional superstructures. On the other hand, mobile particles can diffuse in the volume. The phenomenon of surface diffusion of repulsively interacting adsorbates diffusing in a periodic potential is of great importance regarding catalysis, corrosion and crystal growth problems [8,9] where the dynamic of diffusion process is strongly influenced by the formation of ordered regions.

In general, phase transitions are described within statistical thermodynamic approach [10] or by Monte Carlo method [11]. The latter picks up all possible situations. However, the understanding of the phenomenon and the interpretation of the physical effects related to are reached only by analytical treatments. In the case of the order-disorder transition, one introduces short and long range order parameters. Here we consider only short range order parameter as the diffusion process is essentially sensitive to the local order.

One of the most particular quantities that characterises the diffusion process with the establishment of a phase transition for the bi-dimensional systems is the diffusion coefficient [5,12-16]. The latter is a good indicator of the environment in which the mobile particles diffuse. In effect, at the solid-liquid transition, for example, the diffusion coefficient changes by nearly five orders of magnitude. In the case of pre-melting surfaces, the diffusion coefficient of the mobile particles is comparable to the correspondent liquid.

As a first approximation, we consider that the crystalline structure forms a lattice and we use the lattice gas model because it furnishes the easiest description which includes the dynamics of the diffusion and the phase transition. In the case of systems undergoing order-disorder transition, the lattice gas model favours the discrepancy of different overlapping sublattices at a critical concentration that marks the break down of the lattice occupation symmetry. For a square lattice, the order consists in filling one of the two sublattices when the overall particle density is fixed at $\frac{1}{2}$. No doubt, the lattice gas model is a crude approximation as it ignores completely the relaxation effect caused by the interaction between the diffusing particles on the one hand and between the particles and the substrate on the other. This is contested especially at high concentration as the lattice spacing changes because of the relaxation of the substrate leading to the deformation of the surface potential. In addition, the model assumes that the change of the temperature doesn't influence the potential wells. The paper is organised as follows:

In the section II, we present the dynamic of the lattice gas model and derive the coupled kinetic equations that govern the dynamics of the diffusion process in the bi-dimensional systems with the appearance of a $p(2 \times 2)$ structure. In the section III, we discuss the results of the numerical solution of these equations and specify that the evolvement of the system consists in a relaxation towards the static state. Then, we demonstrate that the growth of the available space for the superstructure is a limited process which can be described by a power law. The section IV is reserved to the calculation of the diffusion coefficient. Then, we give a preliminary study of the diffusion front in the presence of interaction.

II. DYNAMIC OF THE LATTICE GAS MODEL

The crystalline surface is modelled by a lattice whom sites coincide with the potential minima available for the diffusing particles. Every site of the lattice can be either occupied or empty and one introduces an occupation number n_i where i is the site label and n takes respectively

* e-mail: fsbcui@mail.cbi.net.ma

the values 1 or 0. The thermodynamic is completely determined specifying the hamiltonian of the system. Here only the static pair interactions are taken into account. The hamiltonian is written as:

$$H = - \sum_{\langle ij \rangle} \epsilon_{ij} n_i n_j - \mu \sum_i n_i \quad (1)$$

where i and j are the nearest neighbouring sites labels, ϵ_{ij} is the pair repulsive interaction energy of the particles at these sites and μ is the "external" chemical potential. To get a good understanding of the meaning of the "external" chemical potential, it is more suitable to consider the analogy between the lattice gas and the magnetic systems. This is easily done by replacing in equation (1) the occupation number by $(1+S_i)/2$ where S_i is the spin of the particle at the site labelled i . In this limit the external chemical potential is seen as the external field that controls the magnetisation (see appendix).

Let the configuration $\{n\} = (n_1, n_2, \dots, n_N)$ denotes the occupation state of every site of the lattice. The evolvement of the lattice gas is due to the change of its configurations. The dynamics is then attributed to the variation of the state of the occupation numbers rather than to the motion of the particles. As we neglect in addition the vibrational motion and the trajectory of the mobile particles, we associate the change of the configurations to the jump of the mobile particles. Hence, the dynamics is defined by the choice of the transition rate between possible configurations. A standard choice is giving by Kawasaki [10] and is relative to the dynamics of spins exchange in a magnetic system. We adopt a quite different expression of the transition rate. Rather than the Metropolis rule, we expect that the jump of the mobile particle is possible once the energy of the particle exceeds the potential barrier ΔE . This is explained by the fact that the diffusion is an activated process and that the particle at the site i feels a local connection energy and an activation one U : $\Delta E = U + \epsilon \sum_{a'} n_{i+a'}$, where a'

joins the site i to its first neighbours. In addition, we assume that the system is in contact with a reservoir. For a thermal energy deeper than the potential height, the transition rate for the jump of a particle from i to j sites obeys to the Arrhenius law:

$$\omega_{ij} = \nu_o \exp(-\beta \Delta E) \quad (2)$$

where ν_o is the frequency of the vibrational motion of the particles at the bottom of the potential well and $\beta = 1/k_B T$ with k_B is the Boltzmann factor and T is the temperature. We can introduce the constant $\omega_o = \nu_o \exp(-\beta U)$ which gives the time scale. Hence, the transition rate is written as a function of the energy difference between the departure site and the saddle point taken at a fixed energy independent of the sites state. With the present choice of the weight of the transition frequency the calculation lead

to the Boltzmann equilibrium distribution. The transition frequency can be written as:

$$\omega(\{n\}, \{n'\}) = \sum_{ij} \omega_{ij}(\{n\}) n'_i (1 - n'_j) \delta_{n_j n'_i} \delta_{n'_j n_i} \delta_{\{n\}, \{n'\}}^{ij} \quad (3)$$

where the last Krönecker symbol is referred to two configurations different by the jump of an only one particle, $\delta_{n_j n'_i} \delta_{n'_j n_i}$ denotes the permutation of the occupation numbers of the sites i and j and the product $n'_i (1 - n'_j)$ ensures the hard core exclusion condition which defends the double occupation of a same site.

It's clear that the transition frequency ignores the state round the arrival site in the transition rate and does not reflect the whole complexity of the diffusion process. With this choice, we define a stochastic process which is well described by the knowledge of the distribution probability of the configurational space. In effect, to each configuration corresponds a probability of existence at time t : $P(\{n\}, t)$. The time evolution of this probability determines the dynamics of the lattice gas model. Here, we consider that the dynamics is governed by the following master equation:

$$\frac{\partial P(\{n\}, t)}{\partial t} = \sum_{\{n'\}} \left[\omega(\{n'\}, \{n\}) P(\{n'\}, t) - \omega(\{n\}, \{n'\}) P(\{n\}, t) \right] \quad (4)$$

Eq. (4) is a phenomenological one which favours the establishment of the desired configuration. Its stationary solution must lead to the equilibrium distribution

$$P_{eq}(\{n\}) = \frac{1}{Z} \exp(-\beta H) \quad (5)$$

where Z is the partition function.

Hence, the transition frequency has to satisfy the detailed balance condition which is written as:

$$\frac{\omega(\{n\}, \{n'\})}{\omega(\{n'\}, \{n\})} = \frac{P_{eq}(\{n'\})}{P_{eq}(\{n\})} \quad (6)$$

In the present work, we are mainly interested by the average concentration defined as:

$$p(i) = \langle n_i \rangle = \sum_{\{n\}} n_i P(\{n\}, t) \quad (7)$$

Its time evolution introduces naturally a density of current that represents the balance of jumping particles between the link $i \leftrightarrow j$.

$$\frac{\partial p(i)}{\partial t} = - \sum_{a=j-i} \langle J_{ij}(\{n\}) \rangle \quad (8)$$

with $J_{ij}(\{n\}) = \omega_{ij}(\{n\})n_i(1-n_j) - \omega_{ji}(\{n\})n_j(1-n_i)$.

As one remarks, the kinetic equation that is the derivative of the one point correlation function includes the two points correlation function. In order to encounter this difficulty, we consider the mean field treatment (see appendix). Even though this approximation cannot describe correctly the statics of the system, it constitutes the most easiest way to deal with dynamical calculations. Within the mean field approximation, the density of the current takes the form:

$$J_{ij}(\{n\}) = \omega_o \prod_{a'} \omega_r(p(i+a'))p(i)(1-p(j)) - \omega_o \prod_{a'} \omega_r(p(j+a'))p(j)(1-p(i)) \quad (9)$$

where $\omega_r(p(i)) = \langle \exp(\gamma n_i) \rangle$ is the contribution of the occupation of the site i to the jump probability and $\gamma = -\beta \varepsilon$.

The choice of the expression of the transition rate has been done with some arbitrariness that we use to consider averages which agree with the usual thermodynamics:

$$\omega_r(p(i)) = \exp(\gamma p(i))$$

As indicated, the order-disorder transition is signed by the break down of the lattice occupation symmetry leading to overlapping sublattices that are distinguished by different upper indexes (say A and B for the square lattice). Hence, the evolution of the average concentration of each sublattice of the square lattice is governed by the kinetic equation (8) where upper indexes are introduced:

$$\frac{\partial p^\alpha(i)}{\partial t} = - \sum_{a=j-i} \langle J_{ij}^{\alpha\beta}(\{n\}) \rangle \quad (10)$$

where $\alpha, \beta \in \{A, B\}$ and the density of the current denotes the balance of the particles jumps between the A and B sublattices:

$$\langle J_{ij}^{AB}(\{n\}) \rangle = \varpi^{AB} p^A(i)(1-p^B(j)) - \varpi^{BA} p^B(j)(1-p^A(i)) \quad (11)$$

Where $\varpi^{AB} = \omega_o \prod_{a'} \omega_r(p(i+a'))$

The numerical computations do not show any chaotic regime as the sites of the sublattices are coupled and evolve simultaneously [13]. Due to this property, it is convenient to define at a same site the average concentration of the two sublattices. Hence, the dynamics of the diffusion process is governed by the coupled kinetic equations relative to the evolution of the local average concentration $\bar{p}(i) = (p^A(i) + p^B(i))/2$ and the local order parameter $\eta(i) = (p^A(i) - p^B(i))$.

With the use of equations (10) and (11) one obtains:

$$\frac{\partial \bar{p}(i)}{\partial t} = - \sum_a \langle J_{ij}^{AB}(\{n\}) + J_{ji}^{BA}(\{n\}) \rangle \quad (12a)$$

$$\frac{\partial \eta(i)}{\partial t} = \sum_a \langle J_{ji}^{BA}(\{n\}) - J_{ij}^{AB}(\{n\}) \rangle \quad (12b)$$

For a centro-symmetric lattice, the equation (12a) is transformed into a conservative equation :

$$\frac{\partial \bar{p}(i)}{\partial t} = - \frac{1}{2} \sum_a D_a J_{i-a,j}^{\alpha\beta} \quad (13)$$

where $D_a f(i) = f(i+a) - f(i)$ is a difference operator.

III. DYNAMICAL TRANSITION AND TENDENCY TOWARDS EQUILIBRIUM

The numerical solution of the equations (12) shows that the dynamics of the diffusion process in systems undergoing order-disorder transition is characterised by the break down of the lattice occupation symmetry at a critical concentration. This corresponds to a non vanishing but slight value of the order parameter. Then, we assist to the establishment of a transitory regime where the relaxation of the order parameter is extremely rapid (fig.1a). In this transitory regime, there is a progressive localisation of the mobile particles near the source which can be easily identified in the representative curve of the diffusion profile (fig.2a).

For times greater than a certain critical one t_c , all the density profile curves merge to an invariant profile when the average concentration is represented as a function of the reduced variable x/\sqrt{t} as indicated in the figure 2b. This is the second regime - the stationary one - where the increase of the amplitude of the order parameter becomes slower before reaching its maximal value. Moreover, this steady state regime is characterised by the growth of the width of the order parameter curve. The latter process is well discussed in ref. [16] where the purpose of the study concerned the approach of the system to its equilibrium state. The consideration of the tendency of the system towards the equilibrium is suggested by the easily distinguished saturation of the maximal value of the order parameter.

The equilibrium order parameter is obtained from the phase diagram for a given reduced energy γ . We recall that the static curve is obtained by canceling the current along the link $i \leftrightarrow j$ in an homogeneous medium and by fixing the chemical potential associated with a given temperature at a fixed average concentration.

We then conclude that the dynamics of the bi-dimensional lattice with an eventual appearance of a $p(2 \times 2)$ structure consists in a transitory regime marked by the rapid relaxation of the order parameter and a stationary one.

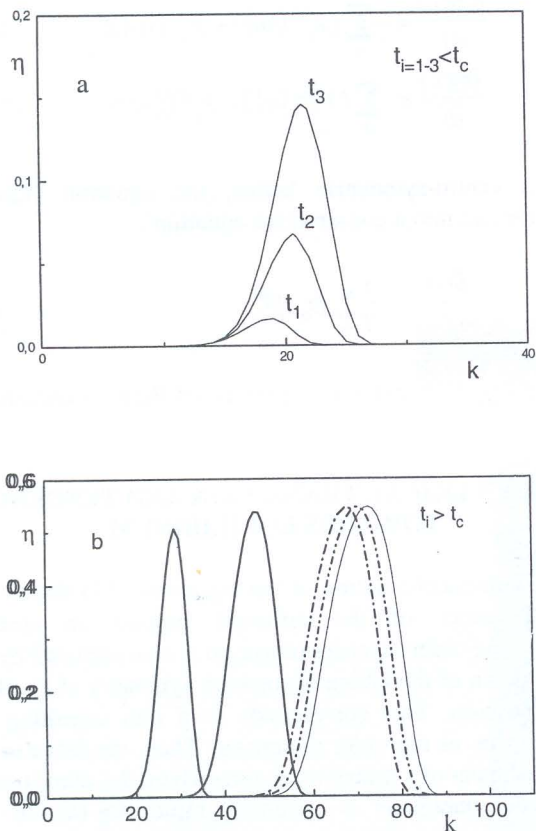


FIG. 1: The relaxation of the order parameter for the square lattice for both times less and greater than the critical one. In the figure 1a, we assist to the rapid relaxation of the order parameter. In the second figure, the relaxation process is slower and leads to the saturation of the maximal value of the order parameter.

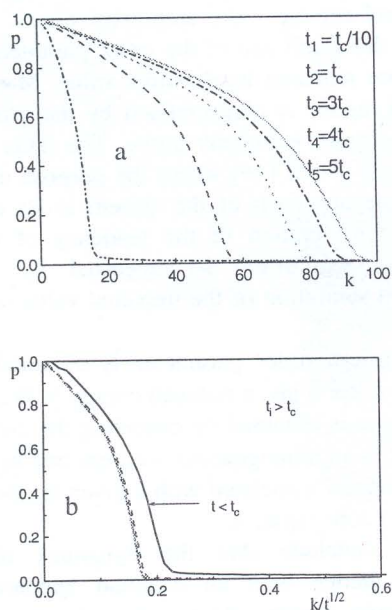


FIG. 2: The density profile for times less and greater than t_c (fig.2a) and its scaling behaviour (fig. 2b).

Considering the second regime, the evolution towards the static behaviour is presented in fig. 3a where are plotted curves of the slower relaxation of the order parameter.

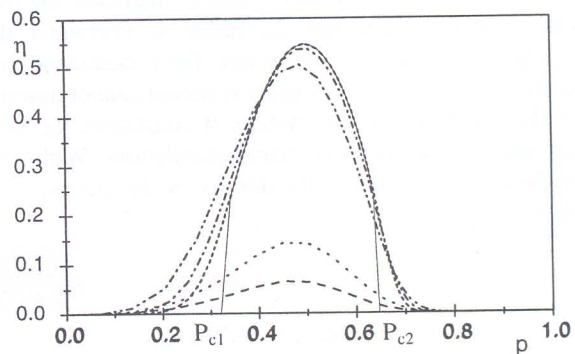


FIG. 3a: The evolution of the system towards the static state

We notice that these curves do merge. Hence, the dynamics of the steady state of the considered driven diffusive system can be mapped on the static state except round critical concentrations p_{c1} and p_{c2} .

One normally compare the dynamical behaviour of the order parameter to the statical one, especially to specify the critical points. The worry isn't justified when knowing that these singular points correspond to the maximal values of the derivative of the order parameter i.e. the dynamical order parameter does inform on these particular points by presenting in them its maximal slopes. In fig. 3b, we report the time dependency of the maximal slopes and show that their behaviour is well fitted by the following power law:

$$\left(\frac{d\eta}{dt} \right)_{\max} \propto t^{-1/3} \quad (14)$$

From the above results we deduce that the order-disorder transition rises by the break down of the lattice occupation symmetry which is accentuated more and more by the filling of one sublattice leading to the growth of the ordered structure. The regime is qualified transitory as the relaxation of the order parameter is, as already mentioned, extremely rapid. When this relaxation process becomes slower, we assist to an increase of the width of the order parameter curve (see fig.1b).

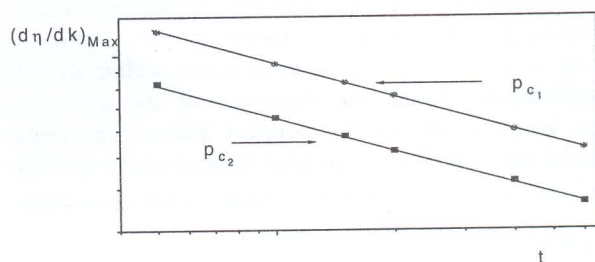


FIG. 3b: The time evolution of the order parameter slopes and the power law dependency showed in a log-log plot.

Let's define the width at half maximum of the order parameter " $\sigma(L, t)$ " as the available space for the growth of the $p(2 \times 2)$ ordered structure. As the dynamical behaviour of the system in its steady state consists in a tendency to the statics, the introduced available space is limited and saturates when reaching the width at half maximum of the static order parameter. Owing to this, the growth phenomenon is limited as well. We propose to describe this growth process by scaling relation of type:

$$\sigma(L, t) = L^\alpha f(t/L^z) \quad (15)$$

where L is the lattice size and f is a scaling function hence defined:

$$f(x) = \begin{cases} x^\beta & \text{if } t \ll t_c \\ \text{cste} & \text{elsewhere} \end{cases} \quad \text{with } \alpha = \beta z$$

It is important to notice that the considered scaling law is different from the dynamic scaling one which introduces the lateral size of the system. Here L is the size of the system in the diffusion direction. By reporting the obtained results on a log-log plot (fig.4), we confirm that the steady state is characterised in particular by the limited growing process of the ordered structure which is well fitted by the scaling relation with the exponents $\alpha = 0.62 \pm 0.05$ and $z = 1.44 \pm 0.03$.

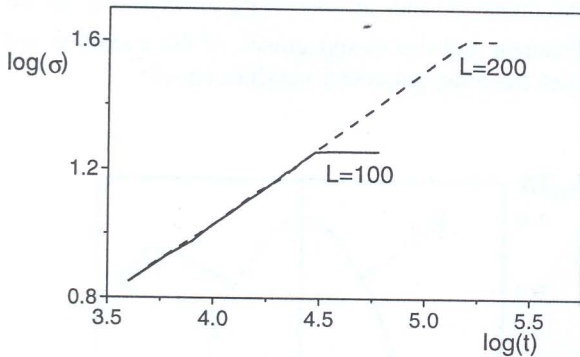


FIG. 4: the representative curve of the saturation of the available space for the growth of the ordered structure.

IV. THE DIFFUSION COEFFICIENT

As mentioned above, the diffusion coefficient is a precious indicator of the environment in which particles diffuse. One has to calculate the chemical, jump and tracer diffusion coefficients D_{coll} , D_j and D^* respectively in order to characterise the diffusion process of strongly interacting particles on the bi-dimensional system. We are interested to the chemical diffusion coefficient that informs on the co-operative effects as it takes into account the local concentration. Its analytical expression is given by the Kubo-Green formula [12]:

$$D_{\text{coll}} = \frac{1}{2\langle(\delta N)^2\rangle} \int_0^\infty \langle \sum_{i,j=1}^N \langle v_i(0) v_j(t) \rangle \rangle dt \quad (16)$$

where $\langle(\delta N)^2\rangle$ denotes the mean square fluctuations of the particles number and the term between brackets is the velocity correlation function.

This equation can be rewritten in terms of a thermodynamic factor associated to the density fluctuations:

$$\frac{\langle(\delta N)^2\rangle}{\langle N \rangle} = \left(\frac{\partial(\mu/k_B T)}{\partial \log(p)} \right)^{-1} \quad (16a)$$

This factor designates the desorption isotherms slopes. Hence, the chemical diffusion coefficient takes the form:

$$D_{\text{coll}} \propto \frac{\partial(\mu/k_B T)}{\partial \log(p)} \quad (16b)$$

This Darken relation considers both the local density fluctuations and the global mean square displacement of the adatoms. By using equation (16b), we derive the following expression:

$$D_{\text{coll}} = p \left[2z' \gamma - \frac{2}{p^A(1-p^A)} + \left(-z' \gamma + \frac{1}{p^A(1-p^A)} \right) \frac{d\eta}{dp} \right] \quad (17)$$

where z' is the number of the occupied nearest neighbouring sites.

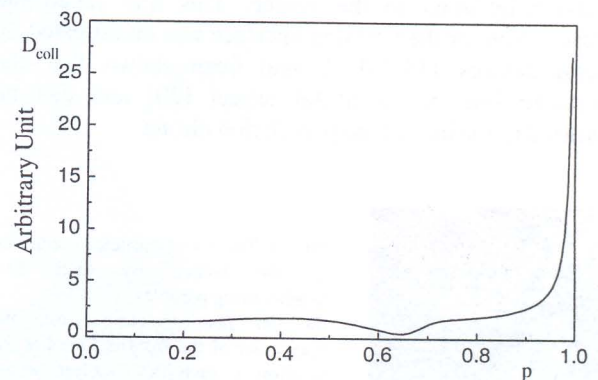


FIG 5a: The collective diffusion coefficient calculated by the Darken relation within the mean field approximation.

In the figure 5b we report the effective diffusion coefficient which is calculated by applying the quasi-stationary approximation, i.e. by considering the statical regime where the density of the current can be developed into a Taylor set and the dynamical order parameter is replaced by the statical one such as the derivative of the order parameter versus the average concentration change suddenly at the critical points. This is not the task in the present investigation which introduce the long time

behaviour of the order parameter rather than the statical one.

By comparing to the collective diffusion coefficient, one notices that the global behaviour of the diffusion coefficient is reproduced in figure (5a) but the method overestimates the critical region. This is due to the carelessness of the gradient contribution in the expression of the chemical potential and to the inclusion of the dynamical order parameter slopes that never diverge.

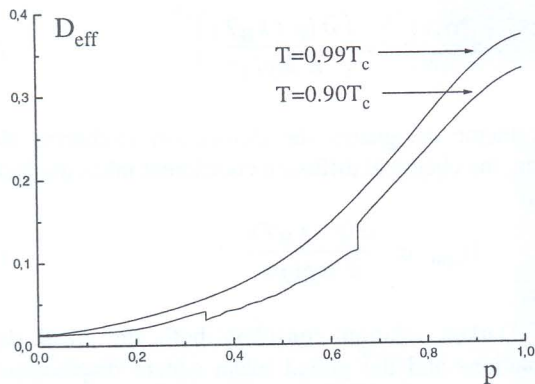


FIG. 5b: The effective diffusion coefficient calculated in the limit of the mean field and the quasi-stationary approximations (From ref. [16])

V. A PRELIMINARY STUDY OF THE DIFFUSION FRONT IN THE CASE OF INTERACTING PARTICLES

One of the most interesting property of the studied system concerns the set of particles connected by their nearest neighbours to the source. This line called the diffusion front or the wedding interface was investigated by several authors [18-23]. It had been shown that the mentioned line has a fractal aspect [20] and can be identified to the hull of the percolation cluster.

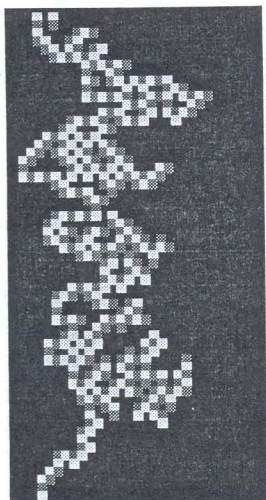


FIG. 6: The set of particles connected to the source by their first neighbouring particles.

In the non-interacting case, the barycenter of the front is found at the position x_f such that $p(x_f)=p_s$ where $p_s=0.59$ is the percolation threshold of the square lattice.

In the interacting case, The diffusion front can also be seen as an interface as it delimits disordered region from the ordered one.

Its features are found universal as both the width and the length were expressed by scaling relations with critical exponents associated to the percolation ones. In addition, the growth of the height of the diffusion front has been characterised by the dynamic scaling [18]. In this paper, we are not interested by the dynamics of the formation neither the fluctuations of the front. Our preliminary study is limited to the effects of the break down of the lattice occupation symmetry on its location. We recall that for the non-interacting case, the diffusion process is described by the second Fick's law and that the average density is given, for the adopted external conditions, by the complementary error function.

The method used here to distribute the profile on the lattice is the same as in reference [13]. To each site of the square lattice, we associate at random a positive value less than one. The value is then compared to the one of the density profile at the same abscissa obtained by solving the coupled kinetic equations (12a) and (12b). The result of the comparison defines the occupation state of the lattice sites.

In the non-interacting case, the value of the concentration of the barycenter x_f of the diffusion front is found closed to the percolation threshold p_s . In addition, the front is of fractal aspect up to a distance σ_f centred around the x_f . Hence, the features of the diffusion front do include critical exponents which are expressed in terms of the percolation ones. In the interacting case, the barycenter of the front must take into account the break down of the lattice occupation symmetry at a certain concentration and the presence of an ordered structure. For this reason, we had calculated for different interaction values the critical concentrations p_{c_1} and p_{c_2} associated respectively to the establishment and the disappearance of the transition and for which the order parameter vanishes ($\eta \rightarrow 0$).

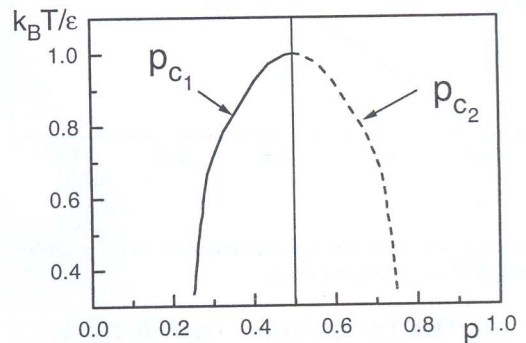


FIG. 7: The phase diagram obtained from the solution of the equations (12) in the limit of weak value of the order parameter.

The resulting phase diagram is shown in figure 7. One easily realises that the position of the diffusion front barycenter for temperatures less than the critical one T_c must be influenced by the existence of the ordered structure. This can be seen by varying the concentration for a given reduced temperature less than one. The barycenter of the front has cannot be placed at the percolation

threshold as the abscissa for $p=0.59$ is embedded in the ordered region. This time, the diffusion front acts the part of the interface delimiting ordered and disordered regions. More details about this part will be given in a future publication [24].

VI. CONCLUSION

In this study, we consider a simple example of driven diffusive system that is a system of repulsively interacting particles submersed in a crystalline regular potential and constraint to diffuse under the action of a concentration gradient. We show that the driven diffusive systems generally pass through a transitory regime that leads to the establishment of a stationary state. In this example, the transitory regime corresponds to the break down of the lattice occupation symmetry and to a rapid relaxation of the order parameter. The second regime is the one relative to a slowest evolution of the order parameter that leads to the saturation of the width of the available space for the growth of the ordered structure. The tendency towards the static state and the saturation of the growth process are described by power laws.

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APPENDIX A: ANALOGY BETWEEN THE LATTICE GAS AND THE SPIN SYSTEM

In the lattice gas formulation the static interactions between first neighbouring particles are considered by the following hamiltonian:

$$H = -\varepsilon \sum_{ij} n_i n_j - \mu \sum_i n_i \quad (A1)$$

where the minus sign in the first right hand term designates that $\varepsilon > 0$ corresponds to an attractive energy. μ is the external chemical potential. For a fixed number of particles, the second right hand term is constant and μ can be chosen arbitrarily. In the opposite case, i.e. when the system exchanges particles μ is the parameter that controls the mean number of particles. The analogy with the Ising model is obtained by applying the following relation $n_i = (1 + S_i)/2$ which leads to the Ising form of the Hamiltonian:

$$H = -J \sum_{ij} S_i S_j - h \sum_i S_i + \dots \quad (A2)$$

where $J = \varepsilon/4$ and $h = \mu + 4\varepsilon$.

One sees that the chemical potential of the lattice gas model acts the part of the external magnetic field of the Ising model. We must specify however that the control parameters are different. In the Ising model we control the external field. The magnetisation is given by the minimum of the free energy while for the lattice gas model we control the composition and the chemical potential is deduced from the free energy.

APPENDIX B: MEAN FIELD APPROXIMATION

The mean field approximation can be found in several publications. We present it only to show that it leads to an expression of the free energy similar to the one obtained by Ginzbourg-Landau.

It is well known that the approximation ignores the correlation and pretends that every particle is submersed into the molecular field of its nearest neighbours. The method certainly leads to insufficient statical results but it is the simplest method that allows a primary understanding of the studied phenomenon. The investigations using the other methods can be considered as a gain of the precision in the results.

For calculating the energy in the case of the mean field approximation we just replace the occupation numbers n_i by the average concentration at the same site p_i .

$$E = -\varepsilon \sum_{ij} p_i p_j - \mu \sum_i p_i \quad (B1)$$

This expression can be rearranged by introducing the term $p_{ij} = (p_i - p_j)^2$.

With the usual expression of the entropy and a fixed chemical potential the free energy is written:

$$F = \sum_i \left[\left(\frac{\varepsilon}{4} \sum_a p_{ij}^2 \right) + f(p_i, T) \right] \quad (B2)$$

where f is the local density of the free energy.

Hence, One notices that the equation (B2) is exactly the discrete form of the Ginzbourg-Landau free energy.

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