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LETTER TO THE EDITOR

Interface widths of a moving front in a model of stochastic transport in two dimensions

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Abstract. A discrete lattice model is introduced to study wetting and interface growth using computer simulation. A fraction of the lattice sites are occupied by particles which are in constant stochastic motion and carry charges and wetting fluid from one end of the sample, connected with a source, to the opposite end, connected with a sink. Initially, all lattice sites are dry and all particles are neutral except those in contact with the source, from where both charge as well as wetting fluid spread in the bulk. In this model, the width of the interface between the dry and wet phases seems to grow with time with a power-law exponent which is about $\frac{1}{3}$ in two dimensions, in agreement with theory of growing interfaces. Growth of the charge-density interface width is found to be diffusive. Both the wetting front and the charge-density front move with a non-diffusive power-law exponent.

Because of its diverse applicability, the study of interfaces and wetting has been one of the most active areas during the past several years in statistical physics [1-7]. In most theoretical studies, one usually considers model Hamiltonians such as the discrete Ising model and the ϕ^4 model among phenomenological models [2, 3] to take into account pertinent details to analyse the kinetics of wetting and interface in static thermodynamic equilibrium. Extensive computer simulations [6] have been recently used on a ferromagnetic Ising model to understand the dynamics of the wetting front and the universality of the interfacial amplitudes. Using the Ising model, one studies the formation of an interface between two dissimilar species say, A (described by spin up) and B (spin down), in thermal equilibrium with various constraints of specific situations. However, the Ising model in thermal equilibrium cannot capture all the essential features of non-equilibrium transport. For example, in an immiscible fluid mixture, particles of type A and B are in constant stochastic motion and, as a result of interaction among the particles and transport mechanism, a variety of interfaces may evolve. To illustrate this point let us consider a mixture of particles (A and B) in a sample which is connected with a source (heat, charge and fluid reservoir, etc) at one end and with a sink at the other. The content of the source is transported by only one component (A particles). The source can simultaneously supply more than one quantity, say colour and charge (or immiscible fluid and charge, heat and charge, etc),

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which can be transported via A particles. These particles, charged at the source, can exchange their charge with their neighbouring particles and at the same time these charged particles can colour all the sites along their path, which emerges from the source and ends at the sink. Initially, sharp interfaces of colour and charge density appear and their corresponding widths begin to grow as a function of time. It would be interesting to study the growth of such interfaces as an example of dynamic wetting which cannot be described by equilibrium models. To our knowledge, we attempt here for the first time to study the growth of the interface in a dynamic system (wetting percolation) where we address the evolution of the interface and wetting of two kinds. For studying such interfaces we describe, in the following, a model which may further illustrate a wide applicability in a variety of non-equilibrium systems including the interface [8-12] of various growth models and pattern formation.

Let us consider a two-dimensional lattice of size $L_x \times L_y$ in which mobile particles of type A are randomly distributed [13] with concentration p. Thus, a fraction p of the lattice sites is always occupied by these particles while the rest, a fraction $(1-p)$, is always empty; we call these empty sites 'holes', referred to as B particles above. Now we extend and modify the model introduced by Sapoval *et al* [14] in a percolation study, by including interactions beyond the hardcore. Here particles interact with each other with a repulsive interaction and with holes with an attractive interaction; both particle-particle and particle-hole interactions have the same range (first-neighbour, second-neighbour, ..., nth-neighbour). No two particles can ocupy the same site. Particles and holes can exchange their position but with a constraint of change in energy (see below). One end of the sample, say the left side, is connected with a source (which may be a heat bath, charge reservoir, fluid, etc) while the other end, the right side, is connected with a sink. Now, whenever a particle is in contact with the source it is charged with unit charge density while it is discharged to zero charge density on contact with the sink. These particles also exchange their charge densities with certain frequency f ($f=\frac{1}{2}$, which means that the probability of hopping is equal to that of the charge exchange and this frequency remains fixed for our study here). Thus, charge is transported from source to sink via stochastic motion of the particles. This system may be called a special three-state lattice gas model because of three charge densities (see below).

To study wetting, growth and formation of an interface we assume that, in addition to charge, the source at the left end is connected with a reservoir of fluid which can flow along the path of its carriers, i.e. the charged particles. One may then address questions such as how does the charge-density gradient evolve with time and how does fluid flow from source to sink? This requires us to define a dry and a wet site. A site is dry as long as it is not visited by a particle of unit charge density and it gets permanently wet as soon as a particle of unit charge density hops on it. Particles with unit charge density have everlasting capacity to wet a dry site permanently until they evaporate (are discharged) on contact with the sink, leaving a 'slug-wet-trail'. This may be a very crude idealisation of non-equilibrium wetting in a liquid-vapour mixture and may be useful in understanding stochastic growth models [8-12]. Initially, the whole lattice is dry except the left-most column connected with the source. Although all particles are in constant stochastic motion, the only particles which can wet a site are those which are or have been in contact with the source. Thus, the fluid percolates along the trajectories of the particles of unit charge density and an interface appears between the dry and the wet phase. Here we attempt to understand the growth of the interface and the motion of the front.

Let us now describe the technical details of the hopping mechanism of a particle. First, we set the range of interaction, say the nth-neighbour range. A particle at site i and one of its neighbouring sites j are then selected randomly. If site j is empty then we calculate the following quantities.

(i) The interaction energy E_0 with particles at site i,

$$E_0 \simeq \rho_i \sum_k \rho_k / r_{ik} \tag{1}$$

where index k runs over all the particles and holes from first neighbour to the nth neighbour, ρ_k is the charge density of the particle ($\rho_k = 0$ or 1) or hole ($\rho_k = -1$) at site k and r_{ik} is the distance between sites i and k; holes act as background charges here.

(ii) The interaction energy E_1 for a configuration in which particle and hole positions are interchanged.

(iii) The change in energy $\Delta E = E_1 - E_0$. If and only if $\Delta E \leqslant 0$ is the new configuration is accepted and the particle is moved from site i to site j. On the other hand if site j is occupied then an attempt to move the particle from site i to site j fails and the particle remains at site i. Each attempt (successful or unsuccessful) is counted in the Monte Carlo time step, and each attempt to move each particle once is defined as one MC step. Although we have considered here charge transport, it can be easily applied to various transport processes mentioned in the beginning.

Since we are looking into non-equilibrium aspects of interface [7, 11, 12] and wetting [6], it is important to analyse the growth at the initial stages carefully. Three kinds of densities are considered here:(I) the particle density (concentration p), (II) the charge density of the particles, the carriers, which is defined as the total charge on all the particles divided by total number of lattice sites, and (III) the wetting density which is defined as the ratio of the number of wet sites to the total number of sites. Initially, both the charge-density profile and the wetting-density profile have the same step functional form. In steady-state equilibrium one would expect the charge-density profile to acquire a constant density gradient, with the density increasing linearly from zero at the sink to one at the source, while the wetting density would assume a constant unit value throughout. Our interest here lies in the behaviour for the times between these two extreme limits.

How do charge and wetting densities evolve with time? To address this question, let us look into figure 1, a typical evolution of density profiles. As in most of the stochastic growth processes, here too an exponential increase of the charge-density $\rho_c(x, t)$ profile seems to emerge. However, the time developments of mean positions of the charge-density and wetting-density $\rho_w(x, t)$ frontiers are found to be faster than diffusion (see below). While there is a remarkable similarity between evolution of charge density $\rho_c(x, t)$ of our model (figure 1(a)) and that of the magnetisation $m(z, t)$ of Mon *et al* [6], it is easy note a sharp contrast in evolution of the profiles of two densities, namely the charge density (figure 1(a)) and the wetting density (figure 1(b)). The difference in evolution of the wetting density considered here and that of the magnetisation [6] indicates that our wetting mechanism is quite different from those studied in thermodynamic systems. We will discuss here the interface widths of both charge-density and wetting-density profiles. A precise evaluation of the interface width and an understanding of the dynamics of the frontier are usually hampered by fluctuations and by the finite size of the systems. For thermodynamic models, the dependence of thermal correlation length on temperature is well understood and therefore, it is relatively easy to estimate the finite-size effects [6]. In our model there

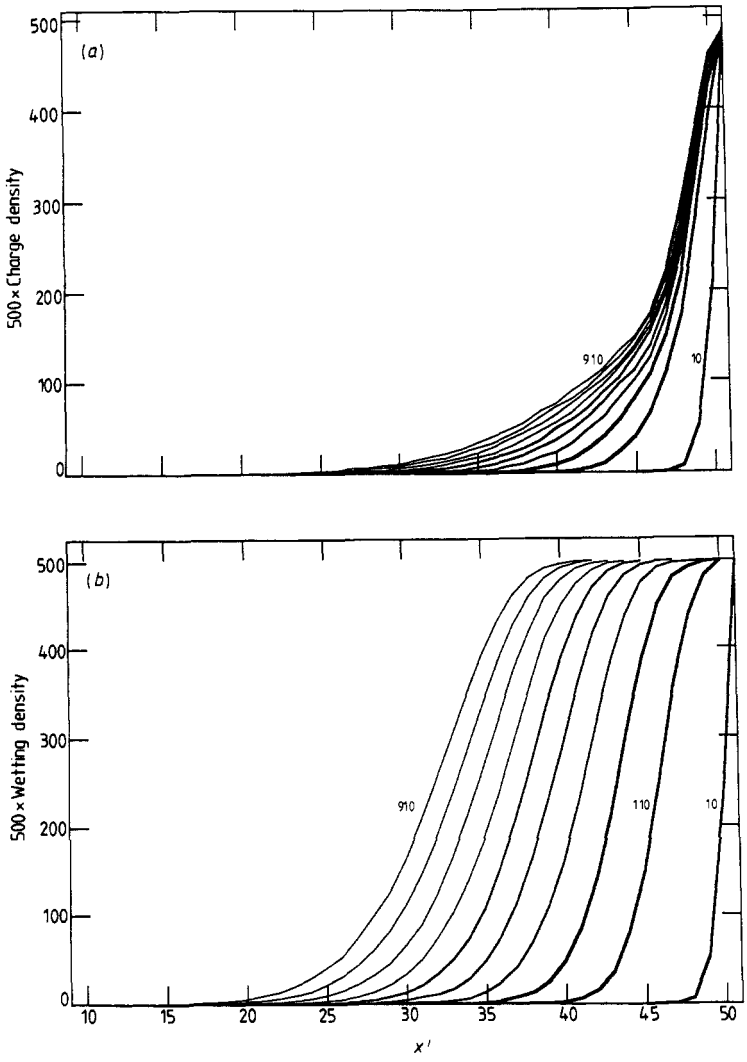

Figure 1. (*a*) Charge density (averaged over column, i.e. $\langle \rho_c(x) \rangle = \Sigma_y \rho_c(y)/L_y$ and (*b*) wetting density (averaged) $\langle \rho_w(x) \rangle$ as functions of distance x' along the x axis from sink at time steps 10, 110, 210, ... , 910 with 500 independent samples on a 50×50 lattice at $p = 0.65$.

are different kinds of fluctuations associated with particle density, particle charge density and wetting density and therefore it is rather difficult to separate the effects of their influence on the interface width and front propagation. However, from the analysis of data for samples of various sizes we get a good estimate for various power laws. When we plot the wetting front and charge-density front positions as functions of time on a semilog scale the qualitative nature of such a plot resembles a similar plot (figure 2) of Mon *et al* [6]. However, we observe a good fit for the front position with time, i.e. with $\langle x \rangle_{\text{front}} \simeq t^k$ when we plot these data on a log-log plot. We find the exponent k to be about 0.70. We also calculate a similar exponent k', also about 0.70 for the RMS displacement of the charge-density frontier. On the whole, our estimates for the power-law behaviour of the moving fronts are quite different from those of

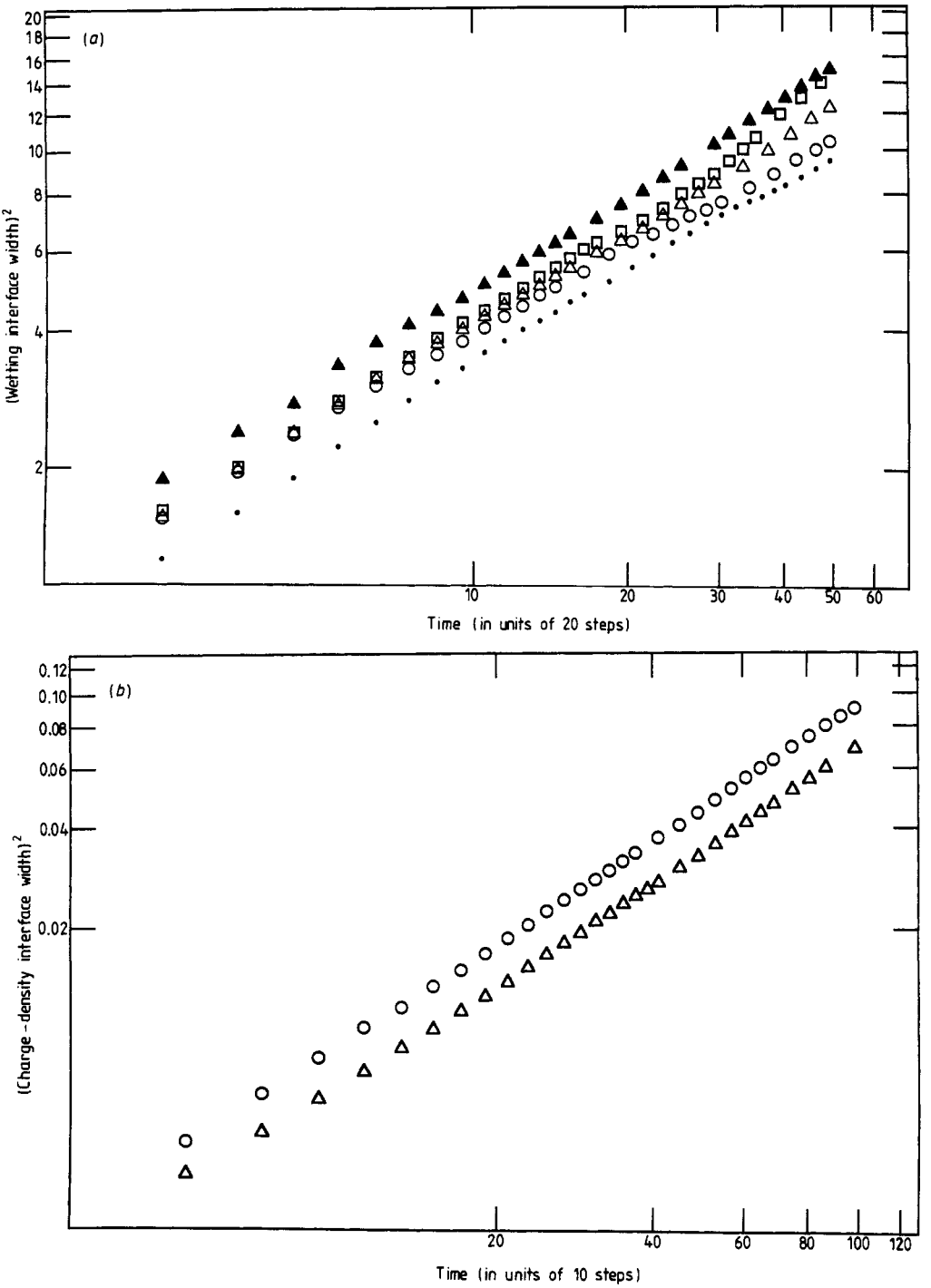

Figure 2. (*a*) (Wetting interface width)^2 plotted against time on a log-log scale. We plot nearest-neighbour interaction at concentrations $p = 0.55$ (500) (▲), 0.65 (500) (△), 0.75 (200) (●) on a 50×50 lattice with runs on additional 50×100 (100) (□) and 50×25 (1000) (○) lattices at $p = 0.65$; the number of samples is in parentheses. (*b*) (Charge-density interface width)^2 plotted against time on a log-log scale for nearest-neighbour interaction at $p = 0.55$ (500) (○), 0.65 (500) (△) on a 50×50 lattice.

their thermodynamic analogue [6] which suggests that the dynamical motion of the wetting frontier in our model may belong to a different universality class than that of the thermodynamic models.

Next, we evaluate the interface widths. First, we locate the position of the wetting frontier, the locus of the last wet site from the source, i.e. for each y direction we find the x coordinates $x_w(y)$ of the last wet site with maximum distance from the source. Calculating the first and second moment of positions, i.e.

$$\langle x\rangle_r = \sum_y x_w(y)/L_y \qquad \langle x^2\rangle_r = \sum_y x_w^2(y)/L_y \tag{2}$$

we estimate the width W_r from

$$W_r^2 = \langle x^2\rangle_r - \langle x\rangle_r^2. \tag{3}$$

Plots of such interface widths for both wetting and charge-density interfaces as functions of time are shown in figure 2. Figure 2(a) shows the variation of the wetting interfaces width with time for several concentrations p of particles with samples of different sizes. For the nearest-neighbour interaction, data with samples 50×100, 50×50 and 50×25 lie very well on the same curve, except for a small deviation in the extreme-time limit where size hinders the growth of the interface. This shows that our data for the growth of the interface is independent of the sample size in a small time range (of interest) after which the front of the interface hits the other end. A log–log fit of the data for the wetting interface width $W \simeq t^{\nu}$, gives us an estimate for the exponent ν to be about $\frac{1}{3}$ for a wide range of the concentrations p of the carriers ($p = 0.10$–0.75). On the other hand, when we increase the range of interaction, we do observe a change in the power-law behaviour of the interface growth. At $p = 0.65$, although there is no significant difference in the power-law behaviour for the interactions ranging from first-neighbour to third-neighbour, incorporating the fourth-neighbour interaction ceases the growth, as the particles are interlocked due to their interactions. It appears that there is an abrupt change in the power-law behaviour of the interface growth as a function of the range of interaction (here on increasing the range from third to fourth neighbour) and this transition should be carefully studied. We also studied the variation of the charge-density interface width with time (figure 2(b)) which shows a power-law behaviour $W_c \simeq t^{\nu'}$, but the exponent ν' is found to be about $\frac{1}{2}$, i.e. the growth of charge-density width is diffusive.

In conclusion, we have introduced a general model to study transport, interface and wetting. We have shown that the motions of charge-density and wetting-density frontiers are non-diffusive. For the nearest-neighbour interacting system the width of the interface formed between dry and wet phases grows with time with an exponent ν found to be about $\frac{1}{3}$, which agrees with the theory [12] of the interface growth exponent in growth models. On the other hand, the growth of the charge-density interface is found to be diffusive. The range of interaction seems to play an important role in governing the motion of the front and growth of the interface width and this aspect should be studied in future.

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