PHYSICAL REVIEW E

STATISTICAL PHYSICS, PLASMAS, FLUIDS, AND RELATED INTERDISCIPLINARY TOPICS

THIRD SERIES, VOLUME 58, NUMBER 1 JULY 1998

RAPID COMMUNICATIONS

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Corner wetting transition in the two-dimensional Ising model

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(Received 4 March 1998)

We study the interfacial behavior of the two-dimensional Ising model at the corner of weakened bonds. Monte Carlo simulations results show that the interface is pinned to the corner at a lower temperature than a certain temperature T_{cw} at which it undergoes a corner wetting transition. The temperature T_{cw} is substantially lower than the temperature of the ordinary wetting transition with a line of weakened bonds. A solid-on-solid-like model is proposed, which provides a supplementary description of the corner wetting transition.
[S1063-651X(98)50507-7]

PACS number(s): 64.60.Cn, 05.50.+q, 68.45.Gd

The two-dimensional Ising model is certainly one of the most important models in statistical mechanics. Exact calculation of its free energy as done by Onsager [1] led to studies of other quantities of this model, such as magnetization [2] and correlation functions [3]. Important applications of this model, which are rather far from the original one, i.e., the description of magnetic transitions, are studies of interfacial phenomena. The earliest step in this direction was made again by Onsager, who calculated the surface tension, which is the excess free energy due to the interface-inducing boundary conditions [1]. More recently, it turned out that the two-dimensional (2D) Ising model can be used to study yet another interfacial phenomenon, namely wetting. It has been shown by Abraham [4] that in the 2D Ising model, on the square lattice with a row of weakened bonds [see Fig. 1(a)], the interface is localized at this row but only at sufficiently low temperature. Moreover, there exists the temperature T_w, which is lower than the critical temperature of this model and, therefore, for $T>T_w$ the interface is delocalized. The results, obtained by Abraham and subsequently generalized [5], provide an important theoretical basis for studying wetting phenomena [6,7]. In order to study wetting, we should adopt the lattice-gas interpretation of the Ising model where, e.g., minus (plus) spins describe liquid (vapor) atoms, respectively, and the delocalization of an interface is regarded as a formation of a macroscopic layer of liquid that wets the substrate.

In the present Rapid Communication, we show that the wetting transition is considerably modified in the presence of a cornerlike boundary. To introduce such a geometry, we assume that the liquid is attracted to both the horizontal and vertical substrates [see Fig. 1(b)]. It turns out that such a geometry induces wetting at a much lower temperature than in Abraham's model. Although we do not consider any particular realization, in our opinion, such geometry might also be relevant from the experimental point of view. Our results are obtained by Monte Carlo simulations of the 2D Ising model and analytical considerations of a simple silicon-on-sapphire (SOS) model, which is supposed to mimic the behavior of the interface.

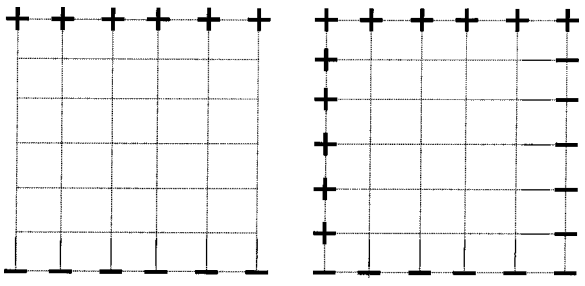

FIG. 1. (a) Geometry of Abraham's model [4]. Top and bottom spins are fixed and there are periodic boundary conditions in the horizontal direction. Weakened bonds are shown as solid thin lines attached to the bottom spins. (b) Geometry of the corner wetting. All boundary spins are fixed at values indicated and weakened bonds are denoted as in part (a).

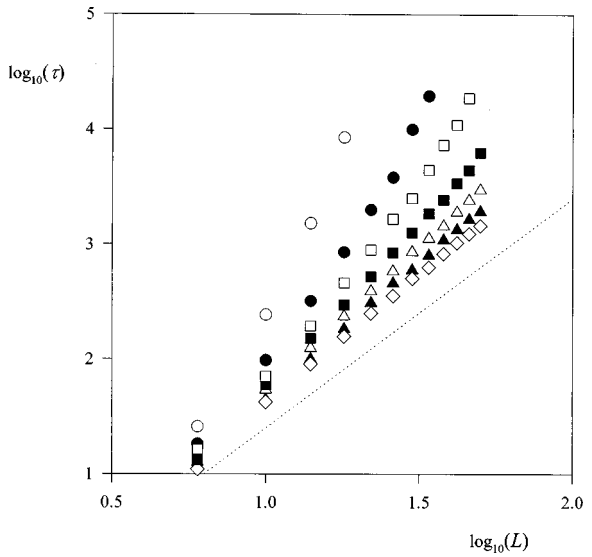

FIG. 2. Size dependence of averaged time τ in the $\log_{10}$-$\log_{10}$ scale. White circles correspond to $T=1.0$, black circles to $T=1.2$, white squares to $T=1.3$, black squares to $T=1.4$, white triangles to $T=1.5$, black triangles to $T=1.6$, and white diamonds to $T=1.7$. For each size L, τ is calculated using data from 10^3 independent runs. The dotted line has a slope corresponding exactly to $\phi=2$.

Let us consider the Ising model defined on the $(L\times L)$ square lattice:

$$H=-\sum J_{ij}S_iS_j, \tag{1}$$

where $S_i=\pm 1$ and $J_{ij}>0$. As direct calculations of equilibrium properties of model (1), with boundaries and interactions as shown in Fig. 1(b), would be rather difficult, we used Monte Carlo simulations. The general behavior of the interface strongly attached to the substrates at low temperatures and delocalized at sufficiently high temperatures is strongly affected by a large relaxation time needed for the interface to delocalize in the macroscopic sense (i.e., over the distance of the order of the system size L). That is the reason that we resorted to the calculation of some dynamical properties of our model. The lattice we consider has all boundary spins fixed as -1. All interactions that link these spins with interior spins have strength J_1, while other interactions have strength $J>J_1$. The initial configuration has all interior spins set to $+1$. We adopted standard Metropolis dynamics in our model [8]. Having all boundary spins fixed to -1, the ground state of the model has all spins set to -1. The main quantity we measured was the averaged time τ needed for the system to reach the state of certain threshold (negative) magnetization (arbitrarily set to -0.5). If the corner wetting transition indeed takes place, the size dependence of τ should have two regimes. At a low temperature the interface should be strongly attached to the (all four) substrates, and as a result, τ should very rapidly increase with the system size L; presumably faster than the power law. Above the corner wetting transition, which takes place at a certain temperature $T_{\rm cw}$, the interface is no longer attached to the substrates and the process of reversing the interior spins should be much faster. The dynamics in this regime should resemble, in our opinion, the ordinary coarsening dynamics in the 2D Ising model. In particular, τ should scale the same way as an averaged time needed for the elimination of a domain of size L. It is well known that such time scales as L^2 [9].

Our Monte Carlo simulations results for L up to 50 and $J_1=0.5J$ are shown in Fig. 2. In the following, J and the Boltzmann constant k_B are put to unity. In our opinion, these results confirm the existence of two temperature regimes with the transition temperature $T_{\rm cw}\sim 1.5$. In particular, for $T\geqslant 1.5$, τ seems to scale as L^{ϕ} with $\phi\sim 2$. Moreover, for $T<1.5$, one can see a systematic increase of the slope, which suggests that τ increases faster than any power of L.

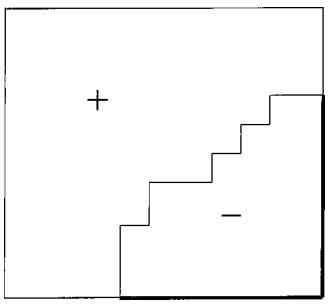

FIG. 3. An example of an admissible configuration of the CSOS model. Thick lines (both of length k) denote regions where the interface, which separates plus and minus regions, is detached from the attracting substrate.

Let us recall that for this model the bulk critical temperature T_c equals $2.2692\cdots$ [1]. Moreover, the ordinary wetting transition temperature T_w equals $1.9585\cdots$, as can be found from the solution of the following equation [4]:

$$e^{2\beta_w}[\cosh(2\beta_w)-\cosh(2j_1\beta_w)]=\sinh(2\beta_w), \tag{2}$$

where $j_1=J_1/J=0.5$ and $\beta_w=1/T_w$. Thus, our rough estimation of $T_{\rm cw}$ shows that the corner wetting transition takes place at a substantially lower temperature than the ordinary wetting transition.

It is generally believed that, although highly simplified, SOS models provide a quite satisfactory description of many interfacial phenomena [7]. In particular, the SOS model of wetting with the pinning potential $v=-2(1-j_1)=-1$ and the elasticity of the interface equal to 2 (we put $J=1$), corresponding to our choice of interactions, has the wetting transition [7] at $T_w^{\rm SOS}=\operatorname{arcsinh}^{-1}(0.5)=2.0781\cdots$, which is quite close to Abraham's result (2) for the Ising model. In the remaining part of our Rapid Communication we introduce a certain corner SOS model (CSOS), which provides an approximate description of the corner wetting transition in our Ising model.

The choice of configurations of the CSOS model is suggested by snapshots of configurations from Monte Carlo simulations of the Ising model, which show that at temperature $T<T_{\rm cw}$ the down spins are located almost exclusively at the corners of the lattice. Thus, we assume that the most relevant CSOS configurations of, e.g., the bottom right corner (see Fig. 3) are specified as follows: (i) the number of columns with nonzero heights is k, where k is the height of the first column (counting from the right in Fig. 3); (ii) the height of the $(i+1)$th column is not greater than the height of the ith column. The first condition is based on the symmetry of the edges of the corner and is chosen for computational simplicity. One can argue that contributions from strongly anisotropic configurations (i.e., when intervals of detachment of the interface from the substrate differ considerably in size) are negligible and relaxing, condition (i) should basically lead to the same results. The height of the first column k is a variable ranging from zero to infinity. The averaged value of k will be determined later using standard prescriptions of statistical mechanics. Since the temperature of the corner wetting transition is very low, we expect that

such a model does provide an accurate description of this transition.

Before we calculate the partition function of this model, let us note that for each configuration of the CSOS model the interface has the same length (we also count the part that is pinned to the boundaries). Thus, in the CSOS model there are no excitations that would increase the length of the interface. The energy of a certain configuration depends, however, on k, i.e., on the length of the section in which the interface is detached from the attracting substrate. With these observations, the partition function of our CSOS model can be written as follows:

$$Z_{\mathrm{CSOS}}=\sum_{k=0}^{\infty} e^{-\beta\epsilon_k} g(k), \tag{3}$$

where $g(k)$ is the number of configurations with a given k and $\epsilon_k=4(1-j_1)k$ is the energy of such configurations. The coefficient $g(k)$, which is calculated using elementary combinatorics, has the form

$$g(k)=\sum_{l=1}^{k} \binom{2k-l-2}{k-l}, \tag{4}$$

where the binomial coefficients correspond to the number of distinguishable distributions of $k-1$ non-negative integer numbers such that their sum equals $k-l$ [10] (non-negative numbers are actually differences of heights of consecutive columns). In Eq. (4) l represents the height of the kth column (i.e., the left-most one in Fig. 3), which by definition has to be positive.

Although we cannot evaluate the partition function (3) in the closed form, we can easily find the behavior of our model in the vicinity of the transition, i.e, when dominant contributions to Eq. (3) come from large k [11]. In such a case, a simple analysis shows that the coefficients $g(k)$ have the asymptotic form $g(k)\sim 4^k$ and the partition function can be approximately written as

$$Z_{\mathrm{CSOS}}\sim\sum_{k=0}^{\infty} \omega^k=\frac{1}{1-\omega}, \tag{5}$$

where $\omega=e^{[-4\beta(1-j_1)+\ln 4]}$. Moreover, in this approximation we have $\langle k\rangle=\Sigma k\omega^k/\Sigma\omega^k=\omega/(1-\omega)$, which diverges for $\omega=1$, i.e., at $T=T_{\mathrm{cw}}^{\mathrm{SOS}}=2(1-j_1)/\ln 2$. One can easily see that close to the critical point $\langle k\rangle\sim\epsilon^{-1}$, where $\epsilon=(T_{\mathrm{cw}}^{\mathrm{SOS}}-T)/T_{\mathrm{cw}}^{\mathrm{SOS}}$. Moreover, the specific heat $C=\partial/(\partial T)T^2\partial/(\partial T)\ln Z_{\mathrm{CSOS}}\sim\epsilon^{-1}$. In the ordinary wetting the specific heat is finite at the transition temperature [7].

For our choice of interactions $j_1=0.5$ and $T_{\mathrm{cw}}^{\mathrm{SOS}}=1/\ln 2\sim 1.4427\cdots$. In our opinion, the Monte Carlo results in Fig. 2 are in agreement with this estimation of T_{cw}. Let us note that at the corner wetting transition the system is critical so the kinetics of ordering might change, and at T_{cw} the divergence of τ might be described by the exponent $\phi\neq 2$. This might explain why our data for $T\geqslant 1.5$ are described by the effective exponent ϕ as slightly greater than 2. Most likely, however, such a deviation of ϕ is only the finite-size effect, and for $T>T_{\mathrm{cw}}$ and a larger system size the usual kinetics with $\phi=2$ will settle down.

It might be interesting to note that the corner wetting described above might be regarded as a lower-dimensional analogue of a corner rounding [12] in the same way that wetting is an analogue of roughening [13]. In this context one can mention that the corner-rounding transition has been correlated with the glassy transition in a certain three-dimensional (3D) Ising model [14]. It turns out that in this 3D Ising model for temperatures lower than the corner-rounding transition, the coarsening dynamics does not bring the quenched system to the low-energy crystal phase but rather to the glassy phase. Certain arguments can be provided to show that the mechanism that operates in this 3D model is not effective in lower-dimensional versions of this model [14]. A very rapid increase of time τ, which is presumably exponential with the system size for $T<T_{\mathrm{cw}}$ (see Fig. 2), suggests that extended, cornerlike defects might trap the coarsening dynamics even in two dimensions, which would mean the existence of a glassy phase in such models.

Another important extension of the present study might be an examination of the influence of the gravitational field on the wetting layer. Such a field breaks the symmetry of edges and suppresses the infinite vertical growth of the wetting layer. One would hope that, in a model that takes into account gravity and an interaction with a vertical substrate, one should be able to calculate, e.g., the contact angle in capillaries, a quantity that is usually described only by phenomenological theories [6]. Studies of more realistic models, including 3D extensions, will be done in the future.

This research is supported by KBN Grant No. 8 T11F 015 09. I acknowledge allocation of computer time from the Pozńa Supercomputing and Networking Center.

[1] L. Onsager, Phys. Rev. **65**, 117 (1944).
[2] C. N. Yang, Phys. Rev. **85**, 808 (1952).
[3] T. T. Wu, B. M. McCoy, C. A. Tracy, and E. Barouch, Phys. Rev. B **13**, 316 (1976).
[4] D. B. Abraham, Phys. Rev. Lett. **44**, 1165 (1980).
[5] G. Forgacs, N. M. Svrakić, and V. Privman, Phys. Rev. B **38**, 8996 (1988).
[6] S. Dietrich, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1988), Vol. 12.
[7] G. Forgacs, R. Lipowsky, and Th. M. Nieuwenhuizen, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1991), Vol. 14.
[8] K. Binder, in *Applications of the Monte Carlo Method in Statistical Physics*, edited by K. Binder (Springer-Verlag, Berlin, 1984).
[9] A. J. Bray, Adv. Phys. **43**, 357 (1994).
[10] W. Feller, *An Introduction to Probability Theory and Its Applications* (Wiley, New York, 1957), Vol. 1.
[11] Strictly speaking, we are assuming at this moment that the transition is continuous and $\langle k\rangle$ diverges. Later, it will turn out that the transition, found using this assumption, is indeed continuous but the flaw in the logic remains.
[12] C. Rottman and M. Wortis, Phys. Rep. **103**, 59 (1984).
[13] Such an analogy should be taken with care. In three-dimensional systems wetting and roughening are different phenomena that, in general, take place at different temperatures. However, the analogy might help the reader to place the corner wetting transition among other interfacial transitions.
[14] J. D. Shore, M. Holzer, and J. P. Sethna, Phys. Rev. B **46**, 11 376 (1992).