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First-order wetting transition in $d=2$ systems with short-range interactions: Exact solution

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Introduction of two defect lines, one near a wall and another at a distance L, in the $d=2$ Ising model, results in a rounded first-order wetting transition which becomes sharp as $L \to \infty$. All the thermodynamic properties of this transition can be evaluated exactly. Predictions on the finite-size rounding of first-order transitions are verified and confirmed explicitly.

Since the work of Onsager, a number of models describing second-order phase transitions have been solved exactly.[1] These exactly soluble models have been invaluable in that they provided a solid basis for scaling theories both in the thermodynamic limit and in the case of finite systems. Finite-size scaling[2] in turn is a useful method when no exact solution of the problem is available and one has to interpret results of numerical Monte Carlo and transfer-matrix calculations.

The finite-size scaling theory of first-order phase transitions has progressed in the recent years.[3,4] However, except for the mean-field theory, there are no known models which describe first-order transitions and can be solved exactly for finite-size effects. The aim of this publication is to present such a model.

The system we consider is a modification of Abraham's model,[5] which describes a continuous wetting transition with short-range forces in two space dimensions. The experimentally observed wetting transitions are typically of first order and usually involve also some kind of long-range interactions.[6]

In our model, in which only short-range interactions are present, a first-order wetting transition is rigorously obtained. We also calculate the finite-size scaling form of the free energy and investigate the rounding of the transition. By doing so, we confirm recent predictions on the analytic properties of finite-size free energies close to a first-order transition.[3,7] In what follows, we describe our model and then report the results. (Details of the calculation will be presented elsewhere.)

The model is depicted in Fig. 1. We consider a semi-infinite two-dimensional Ising model. The couplings connecting the substrate (the boundary with all spins down, denoted by a minus sign in Fig. 1) to the first layer (column) are given by $J_1 = a_1 J$, with $0 \le a_1 \le 1$, where J denotes the bulk interactions. The boundary conditions at the Nth layer favor all spins up (denoted by a plus sign in Fig. 1). At a distance L from the substrate an additional column of defect bonds $J_2 = a_2 J$ is placed with $0 \le a_2 \le 1$.

At zero temperature (the temperature T will be expressed in units of k/J and we denote $K = J/kT$, $K_1 = J_1/kT$, $K_2 = J_2/kT$), and provided $a_1 < a_2$, an interface develops and is localized at the substrate. If $a_2 = 1$, this interface, in the limit $N \to \infty$, followed by $M \to \infty$ depins from the substrate at a well-defined temperature T_w. This depinning transition first obtained by Abraham[5] is of second order, with a discontinuity in the specific heat. With $a_1 < a_2 < 1$ and $L < \infty$, the second-order depinning transition from the double defect structure still exists at $T_w(L) > T_w$. However, this transition disappears as $L \to \infty$ [with $T_w(L) \to T_c$, where T_c is the critical temperature of the two-dimensional Ising model]. A new feature develops in the $L \to \infty$ limit: The interface unbinds discontinuously at some temperature T_1. The wetting transition at $T = T_1$ becomes sharp first order for $L \to \infty$, and it is "finite-size rounded" for $L < \infty$, as explained below. These observations are depicted in Fig. 2. (The inset will be discussed later.) The dashed line is the surface tension, or the surface free energy per spin of the regular Ising model, which corresponds to $a_1 = a_2 = 1$. The solid line with a well pronounced cusp at $T_1 \simeq 1.62$ describes the surface free energy f (per spin) of our model with $a_1 = 0.5$, $a_2 = 0.6$ in the $L \to \infty$ limit. The dotted lines are analytic continuations of the solid lines above and below T_1. The solid-dotted curve with the dotted part for $T < T_1$ and solid part for $T > T_1$ corresponds to a model (denoted by A) with $a_1 = 1$, $a_2 < 1$ (and $L = \infty$). There is no wetting transition in this model.[8,9] The other solid-dotted curve in Fig. 2 describes the surface free energy of the Abraham model (model B) with $a_1 < 1$, $a_2 = 1$. It merges smoothly with the Onsager curve at T_w.

For a given value of a_1 (which determines T_w) the first-order transition will take place for $a_1 < a_2 < 1$. For

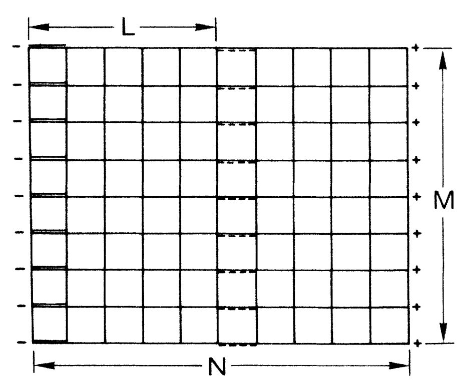

FIG. 1. Definition of the model. Double lines denote $J_1 = a_1 J$, solid-dashed lines denote $J_2 = a_2 J$. All the other couplings are J.

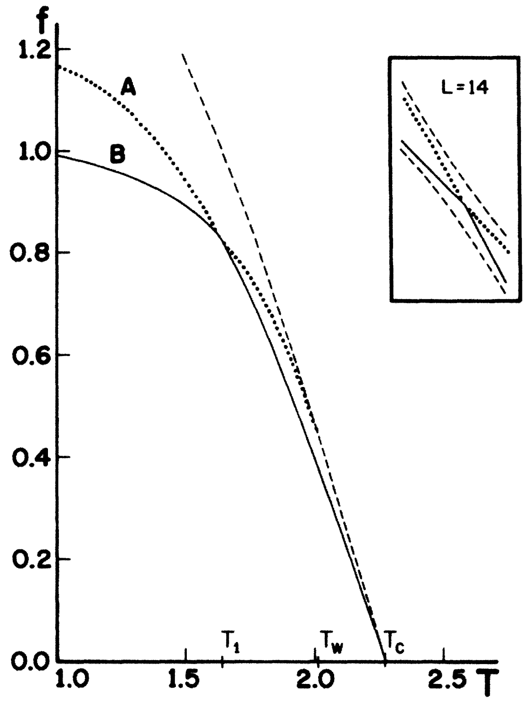

FIG. 2. See explanation of the curves in the text. The sides of the inset rectangle are as follows: Horizontal side denotes T from 1.610 to 1.630, vertical side denotes the free energies from 0.829 to 0.848. The solid and dotted curves correspond to the limit $L=\infty$, while the dashed lines are the two branches of the free energy for $L=14$.

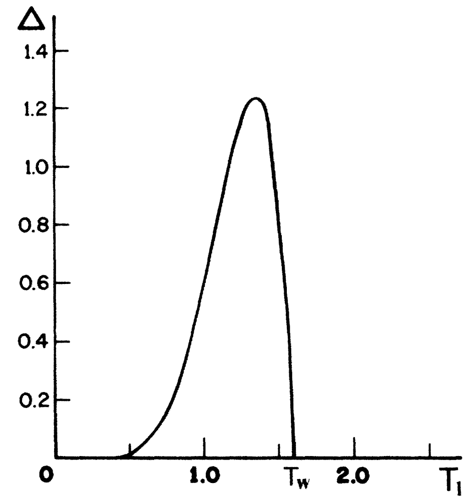

FIG. 3. The jump Δ in the free-energy derivative as a function of T_1. Δ is proportional to the latent heat.

the corresponding value of T_1, we have $0<T_1<T_w$ (in the limit $a_2=a_1$, $T_1\to 0$). At T_1 the first derivative of the free energy with respect to T, which is proportional to the latent heat, has a jump. The variation of this jump Δ with T_1 is shown in Fig. 3 for $a_1=0.72$, $T_w=1.6$.

Since the first-order transition takes place only in the $L\to\infty$ limit, by keeping L finite (but large) we can study the finite-size rounding of this transition. For finite L the free energy is analytic at T_1. As mentioned, for $L<\infty$ there is also an overall continuous depinning transition taking place at $T_w(L)>T_w$, where $T_c-T_w(L)=O(1/L)$. Instead of the two solid-dotted curves of Fig. 2 (describing the free energies f_A, f_B of the models A and B), two branches (dashed lines in the inset of Fig. 2) appear with a gap between them. The value of the gap at T_1 is proportional to $e^{-L/l}$. The expression for l will be given below. The exponential dependence of this gap on L is reminiscent of finite-size scaling behavior of Ising models in cylindrical geometry.[3] Here the full finite-L scaling behavior will be derived in closed analytic form.

To calculate the free energy, we used the transfer-matrix method. The boundary conditions at the vertical edges of the system described in Fig. 1, can be conveniently expressed in terms of a projection matrix, which assumes a simple form upon the application of the Jordan-Wigner transformation.[10] The boundary conditions in the M direction are periodic. Thus, the free energy can be expressed as a trace of an operator which involves a product of the Onsager transfer matrices (with couplings J_1, J_2, J) and the projection matrix. This trace is evaluated in the basis spanned by the eigenvectors of the Onsager transfer matrix. For the surface free energy, in the finite L case, we get

$$-f/T=\lim_{M\to\infty}\frac{1}{M}\ln[1-\exp(-\alpha M|z|^M+\cdots)$$
$$=\ln|z| \ . \qquad (1)$$

where $\cdots$ denote subleading terms for large M. Here α is an unimportant constant, and $z=e^{iq}$ is determined by the following equation:

$$\{[1+\cos q\cos a_q+c^*\sin q\sin a_q](c_1+s_1\cos a_q)+[\cos q\sin a_q+\sin q(s^*-c^*\cos a_q)]s_1\sin a_q\}(c_2+s_2\cos a_q)$$
$$=-e^{-2LE_q}s_2\sin a_q\{(1+\cos q\cos a_q+c^*\sin q\sin a_q)s_1\sin a_q+[\cos q\sin a_q+\sin q(s^*-c^*\cos a_q)](c_1-s_1\cos a_q)\} \ . \qquad (2)$$

The notations in (2) are $c=\cosh 2K$, $c^*=\cosh 2K^*$, $s^*=\sinh 2K^*$, $\tanh K^*=e^{-2K}$, and with $i=1,2$,

$$c_i=\cosh 2(K_i^*-K^*),\quad s_i=\sinh 2(K_i^*-K^*),\quad \cosh E_q=cc^*+\cos q,\quad \tan a_q=\frac{s\sin q}{c^*+c\cos q}\ ; \qquad (3)$$

s in (3) is $\sinh 2K$. The quantity z in (1) is that solution of Eq. (2) the absolute value of which is the closest to unity and at the same time is smaller than unity.

Before discussing the finite L case, let us consider the $L\to\infty$ limit. In this limit we have two factors on the left side of (2). Each can vanish separately, and the corresponding solutions with the same properties as z above are denoted by z_A

and z_B [z_A is the zero of the expression $(c_2+s_2\cos a_q)$]. In terms of z_A and z_B, the surface free energy is given by

$$-f/T=\lim_{M\to\infty}\frac{1}{M}\ln\{1-\exp[-M(a_A|z_A|^M+a_B|z_B|^M+\cdots)]\}=\ln[\max(|z_A|,|z_B|)] \ , \tag{4}$$

a_A and a_B here are unimportant constants; z_A, z_B are functions of T, a_1, a_2. The first-order transition temperature T_1 is determined by $z_A=z_B=z^*$. For $T<T_1$, $1>|z_B|>|z_A|$; whereas for $T>T_1$, $|z_B|<|z_A|<1$. Consequently, in the $L\to\infty$ limit $f=f_B(z_B)$ for $T<T_1$, whereas $f=f_A(z_A)$ for $T>T_1$. If f_A and f_B are extended to the regions $T<T_1$ and $T>T_1$, respectively, then they give the free energies of models A and B. These are the solid-dotted lines in Fig. 2. Solving $z_A=z_B$, we obtain T_1 in terms of a_1, a_2 from the relation

$$\left(\frac{x_1}{x_2}\right)^2=\frac{cs(1-x_1^2)-(c+sx_1^2)}{cs(1-x_1^2)-(s+cx_1^2)} \ . \tag{5}$$

Here, $x_i=\tanh K_i$ $(i=1,2)$. In the limit $a_2=1$, (5) reduces to

$$x_1^2=\frac{s(s-1)}{c(c+1)} \ , \tag{6}$$

which gives $T_w=T_w(a_1)$ for the Abraham transition.[5]

Let us now turn to the finite L case. For large L, close to T_1, Eq. (2) can be conveniently written as

$$(z-z_A)(z-z_B)=Pe^{-2LE_q} \ . \tag{7}$$

Both E_q and the coefficient P are complicated functions of T, L, a_1, and a_2. Here, however, they are evaluated at $L=\infty$ and $T=T_1(a_i)$. Relation (7) determines z correctly in the asymptotic regime $L\to\infty$; $z_A,z_B\to z^*$. Solving (7) for z finally gives the two branches, denoted by dashed lines in the inset of Fig. 2,

$$f_\pm=\tfrac{1}{2}\{(f_A+f_B)\mp[(f_A-f_B)^2+Re^{-2LE_q}]^{1/2}\} \ . \tag{8}$$

Here R is a complicated function of z^*, etc.; f_A, f_B are now defined on both sides of T_1. Relation (8) is, of course, valid only in the vicinity of T_1 and in the limit of large L; f_+ and f_- are, respectively, the lower and the upper branch in the inset. The characteristic length l, introduced before, is given by E_q^{-1}. We did not find any simple interpretation for this length scale. It is certainly not the bulk correlation length (evaluated at T_1). The "mixing" of two branches as a mechanism of finite-size rounding is similar to that predicted phenomenologically[3,7] for Ising models in cylindrical geometries.

In conclusion, we presented the exact solution of a first-order wetting transition, with short-range interactions, in two dimensions. We were able to analyze the finite-size rounding of this transition and for the first time check explicitly the phenomenological finite-size scaling theory.[3,7] One interesting consequence of our analysis is that defects or imperfections far from the wall can drive the wetting transition first order (it will be practically sharp as long as L is large). Unlike other theories of weakly first-order wetting transitions, there is no prewetting line in this case (for $L=\infty$), which is reminiscent of several experimental findings.[6]

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