PHYSICAL REVIEW B VOLUME 15, NUMBER 2 15 JANUARY 1977

Roughening transition in the solid-on-solid model

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(Received 6 May 1976)

It is shown that the failure of the Temkin approximation to predict a roughening transition in the solid-on-solid model is due to the neglect of certain correlations perpendicular to the interface. The inclusion of these correlations is essential to any consistent description of roughening. Taking them into account leads to a divergence of the interface width even within the framework of a mean-field approximation.

I. INTRODUCTION

In 1949, Burton and Cabrera[1] suggested that the width of the interface between two phases in a three-dimensional Ising model should diverge at a "roughening" temperature T_R, which is lower than the bulk critical temperature. Since they were considering this system as a model for the solid-gas interface, the phenomenon of roughening would have a direct application to the theory of crystal growth.[2]

This suggestion has been supported by low-temperature series expansions[3] and Monte Carlo studies,[4-6] but the microscopic description of the roughening transition has not been satisfactory.

In 1966, Temkin[7] used a Bragg-Williams analysis to obtain an approximate description of the solid-on-solid (SOS) model (high-anisotropy limit, described in Sec. II). His results for the thermodynamic properties of the interface are in good qualitative agreement with Monte Carlo data,[4,5] but his failure to find a roughening transition presented a serious problem, since mean-field approximations are usually reliable for predictions of the existence of phase transitions in more than one dimension. The absence of an explanation of why the Tempkin approximation gives a finite interface width at all temperatures cast some doubt on the existence of the roughening transition.

In this paper, we show that the Temkin approximation neglects certain correlations that are essential to an understanding of the roughening transition. The inclusion of these correlations leads to a divergence of the interface width even within the framework of a mean-field approximation. The divergence can be described by roughening exponents,[3] which we also calculate.

In Sec. II, we discuss the relationship between the models of an interface under consideration. We then rederive the naive-mean-field and Temkin results in Secs. III and IV to show why such approximations cannot describe roughening. In Sec. V, we present an approximation that provides a microscopic description of the roughening process.

II. ISING AND SOS MODELS OF AN INTERFACE

We begin with an anisotropic Ising model

$$\mathcal{H}(\text{Ising}) = -\sum_f \sum_g J_{f,g} S_f^z S_g^z - g\mu_B H \sum_f S_f^z \,, \quad (1)$$

with $S_f^z = \pm\frac{1}{2}$. We shall restrict the discussion to nearest-neighbor interactions with positive exchange constants: J in the x and y directions and J' in the z direction. Below T_c, an interface is produced by imposing antiperiodic boundary conditions in the z direction. The free energy associated with the interface is then obtained by subtracting the free energy with fully periodic boundary conditions and taking the thermodynamic limit. An immediate consequence is that the energy (and free energy) of the interface at $T = 0$ is J' for each site in the x, y plane.

In the lattice-gas interpretation used in the theory of crystal growth, a site is said to be occupied if $S_f^z = +\frac{1}{2}$ and empty if $S_f^z = -\frac{1}{2}$. The concentration of particles (up spins) in the nth layer parallel to the interface is then

$$c_n = \langle S_f^z \rangle_n + \tfrac{1}{2} \,. \quad (2)$$

The SOS model, which plays a prominent role in the theory of crystal growth, is simply the high-anisotropy limit $J' \to \infty$. The bulk critical temperature becomes infinite in this limit, as does the free energy of the interface. It is convenient to subtract the (infinite) ground-state energy in the definition of the SOS Hamiltonian:

$$\mathcal{H}(\text{SOS}) = \lim_{J' \to \infty} [\mathcal{H}(\text{Ising}) - E_0] \,. \quad (3)$$

For the theory of crystal growth, we set $J = \epsilon$ and $g\mu_B H = \Delta\mu$ and write

$$\mathcal{H}(\mathrm{SOS}) = \epsilon \sum_i \sum_j \left(|h_{ij} - h_{i,j+1}| + |h_{ij} - h_{i+1,j}| \right) - \Delta\mu \sum_i \sum_j h_{ij}, \quad (4)$$

where i and j are the x and y coordinates and h_{ij} is the height of the surface. We shall restrict further discussion to the equilibrium condition, $\Delta\mu = 0$.

The width of the interface can be measured in several ways.[3] If the ground state of the system is taken to be $c_n = 1$ for $n \leq 0$ and $c_n = 0$ otherwise, then the reciprocal of $(c_0 - c_1)$ provides one measure. Other measures are given by the moments

$$\langle n^{2p} \rangle = \sum_{n=-\infty}^{\infty} n^{2p}(c_n - c_{n+1}), \quad (5)$$

where p is a positive integer.

III. NAIVE-MEAN-FIELD APPROXIMATION

The simplest application of the mean-field approximation (MFA) to the anisotropic Ising model consists of supplying indices to the usual equations[8] to specify the layers involved. For the magnetization in the nth layer $\sigma_n = \langle S_f^z \rangle_n$, we have

$$\sigma_n = \tfrac{1}{2} \tanh[\beta J \bar{z} \sigma_n + \beta J'(\sigma_{n-1} + \sigma_{n+1})], \quad (6)$$

where $\bar{z}$ is the number of nearest neighbors within the x,y plane. In addition to the homogeneous solution $\sigma_n = \sigma$, there exist solutions with the property

$$\lim_{n \to \pm\infty} \sigma_n = \mp |\sigma|, \quad (7)$$

which have been shown to give a plausible description of an interface for $J' = J$.[9] However, naive MFA fails completely in the SOS limit. If $\sigma_{n-1} + \sigma_{n+1}$ is not exactly zero, then $|\sigma_n| = |\sigma| = \frac{1}{2}$ and we have the incorrect prediction of a perfectly sharp interface for all temperatures. The difficulty lies in the neglect of correlations in the z direction (longitudinal correlations). These correlations become increasingly important as J' increases and their neglect leads to an averaged (infinite) interaction with all spins in neighboring layers.

IV. INCLUSION OF LONGITUDINAL CORRELATIONS BETWEEN SPINS (TEMKIN APPROXIMATION)

Fortunately, the longitudinal correlations between spins can be treated exactly in the SOS limit. Table I shows the four configurations of the spins directly above and below a given spin in the nth layer. In cases 1 and 2, the spin is "frozen" and only in case 3 it is free to take on both positive and negative values. Case 4 is forbidden because it would require an additional energy of $2J' = \infty$. For the magnetization of the free spins, σ_n', we again use MFA, so that now

TABLE I. Spin configurations in the SOS model above and below a given site in the nth layer. Case 4 is excluded because it would require an excitation energy of $2J' = \infty$ ($\sigma_{-\infty} = +\frac{1}{2}$ and $\sigma^{+\infty} = -\frac{1}{2}$).

Case	Configuration Above $(n+1)$	Configuration Below $(n-1)$	Concentration in nth layer	$\langle S_f^z \rangle_n$
1	$+\frac{1}{2}$	$+\frac{1}{2}$	c_{n+1}	$+\frac{1}{2}$
2	$-\frac{1}{2}$	$-\frac{1}{2}$	$1 - c_{n-1}$	$-\frac{1}{2}$
3	$-\frac{1}{2}$	$+\frac{1}{2}$	$c_{n-1} - c_{n+1}$	σ_n'
4	$+\frac{1}{2}$	$-\frac{1}{2}$	0 (not allowed)	...

$$\sigma_n' = \tfrac{1}{2} \tanh x_n \quad (8)$$

and

$$x_n = \beta\epsilon\bar{z}\sigma_n = \beta\epsilon\bar{z}(c_n - \tfrac{1}{2}). \quad (9)$$

Combining this with the exact consistency condition (found by combining the last two columns in Table I)

$$\sigma_n = \tfrac{1}{2} c_{n+1} - \tfrac{1}{2}(1 - c_{n-1}) + \sigma_n'(c_{n-1} - c_{n+1}), \quad (10)$$

we find the recurrence relation

$$c_{n+1} = c_n - (c_{n-1} - c_n) e^{2x_n}, \quad (11)$$

which is identical to that found by Temkin[7] using a different method. As Temkin showed, this equation is easily solved by numerical iteration starting from an arbitrary value of $x_1 = -x_0$. The normalization condition in Eq. (7) (with $\sigma = \frac{1}{2}$) determines the corresponding value of the temperature and the full temperature dependence is found by varying x_1. The energy contribution from the nth layer is

$$E_n = \bar{z}\epsilon(\tfrac{1}{4} - \sigma_n^2) = \bar{z}\epsilon c_n(1 - c_n), \quad (12)$$

and other quantities of interest can be calculated using the usual thermodynamic identities.[10] These predictions are in good qualitative agreement with the thermodynamic properties found in Monte Carlo simulations.[4,5]

The iterative procedure is extremely efficient since Eq. (11) converges exponentially. Unfortunately, this also implies that the width of the surface is finite for all temperatures, so that the Temkin approximation fails to predict a roughening transition.

V. INCLUSION OF LONGITUDINAL CORRELATIONS BETWEEN SPIN PAIRS

When spins are frozen into position in the SOS limit and no longer contribute to the thermal properties of the interface, the interactions between such frozen spins are also frozen and do not affect the behavior of the free spins. To take these correlations into account in a mean-field approximation, we need a new expression for the effective field, which contains contributions from interactions with those frozen spins that bound regions containing free spins. To calculate the extent of such boundaries, we introduce the number of antiparallel spin pairs in each layer a_n. The layer energy contribution is then exactly

$$E_n = \epsilon a_n . \tag{13}$$

If we neglect height differences of more than two lattice constants, the number of interactions with boundary spins in the nth layer that are frozen into the plus (minus) one-half state is just a_{n+1} (a_{n-1}).

To approximate the effect of the frozen boundary spins by an external field, we replace Eq. (9) with

$$x_n = \beta\epsilon\sigma_n' \left(\bar{z} - \frac{a_{n+1}+a_{n-1}}{c_{n-1}-c_{n+1}} \right) + \frac{\frac{1}{2}\beta\epsilon(a_{n+1}-a_{n-1})}{c_{n-1}-c_{n+1}} . \tag{14}$$

Note that we have included a correction term to avoid double counting interactions between free spins. Taking this term proportional to $a_{n+1}+a_{n-1}$ gives the correct low-temperature properties, but it is an overestimate due to contributions from height differences of more than two lattice constants. However, this is not crucial to the essential result and the term could be neglected completely (a substantial underestimate) without affecting the existence of the roughening transition. The term proportional to $a_{n+1}-a_{n-1}$ is not affected by height differences of more than two lattice constants.

The layer energy contribution is obtained by the usual MFA method,[8] taking into account the condition that $E_n(\sigma_n' = \pm\frac{1}{2}) = \epsilon a_{n\mp1}$. Equation (12) is replaced by

$$E_n = \epsilon\left[\tfrac{1}{4} - (\sigma_n')^2\right]\left[\bar{z}(c_{n-1}-c_{n+1}) - (a_{n+1}+a_{n-1})\right] - \epsilon(a_{n+1}-a_{n-1})\sigma_n' + \tfrac{1}{2}\epsilon(a_{n+1}+a_{n-1}) , \tag{15}$$

to get a closed set of simultaneous equations, namely, (8), (10), (11), and (13)–(15).

Far from the interface (n large), $x_n = x$ independent of n and, after some algebra, we find

$$x = 2\beta\epsilon \tanh(2x) . \tag{16}$$

This equation has nonzero solutions for x as long as $\beta\epsilon > \frac{1}{4}$. For higher temperatures, only the solution $x = 0$ exists and the recurrence relation (11) shows that the interface width diverges; our new approximation gives a roughening temperature $k_B T_R = 4\epsilon$. As is usual in mean-field approximations, the predicted transition temperature is higher than the best estimates from low-temperature expansions[3] (1.23ϵ to 1.32ϵ) or Monte Carlo simulations (1.15ϵ).[11]

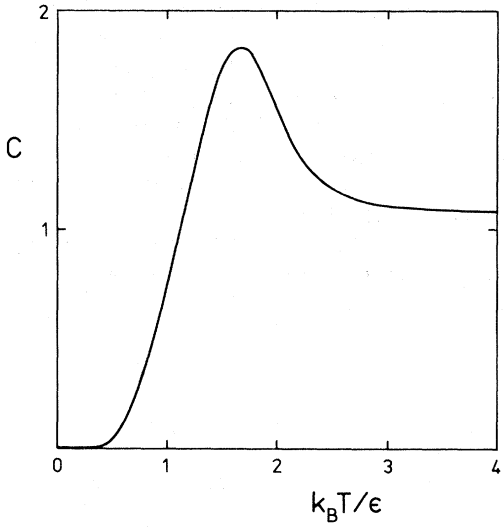

FIG. 1. Interface specific heat as a function of temperature.

To obtain a full numerical solution, we first set $x_n = x$ for all $n > 1$ and then, beginning with $n = 1$, solve the equations for the nth layer, holding the parameters for the other layers fixed. The process is repeated until convergence is found. The procedure is quite fast, except close to T_R, where many layers must be taken into account.

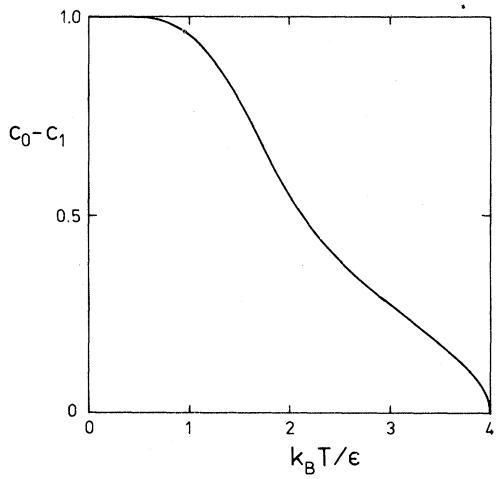

FIG. 2. $c_0 - c_1$ as a function of temperature.

The thermodynamic properties, such as the specific heat shown in Fig. 1, do not show any singular behavior at T_R. These properties are quite close to those found in the Temkin approximation and, at low temperatures, the predictions of the two approximations become identical for all quantities of interest, including the various measures of the width.

As $k_B T \to 4\epsilon$, all measures of the width diverge in the new approximation. Near T_R, we can describe the singularities by "critical" exponents and find that $(c_0 - c_1)$ goes to zero with the square root of $(T_R - T)$ as shown in Fig. 2, $\langle n^2 \rangle$ diverges with the first power, and $\langle n^4 \rangle$ diverges with the second power.

ACKNOWLEDGMENTS

I would like to thank Dr. H. Müller-Krumbhaar, Professor D. P. Landau, Professor H. Wagner, and Dr. J. Harris for interesting and stimulating discussions.

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