Journal of Statistical Physics, Vol. 50, Nos. 5/6, 1988

Interface Delocalization in the Three-Dimensional Ising Model

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Received May 6, 1987; revision received October 6, 1987

The interface delocalization in the three-dimensional Ising model is studied by real-space renormalization group methods. The first-order cumulant expansion approximation is used. Defect free energies for a boundary plane of defects and an internal plane of defects are calculated in the whole temperature region. The phase diagrams are also obtained. The method and the model analyzed may give a correct phase diagram only in the regime of continuous interface delocalization. The interface delocalization is obtained for the boundary defect and also for the internal defect if the systems on two sides of the internal defect plane have a different degree of order. The delocalization transition does not occur in the case of the internal defect plane between two equally ordered systems.

KEY WORDS: Interfaces; interface delocalization; three-dimensional Ising model; real-space renormalization.

1. INTRODUCTION

Critical phenomena near surfaces, interfaces, and defects in various models have been extensively studied recently.[1-4] Abraham[4,5] has analyzed the two-dimensional ($d=2$) Ising model with a line of weakened defect bonds at the boundary of the lattice. It is possible to introduce the interface into this system by taking suitable boundary conditions. At low temperatures, when the energy terms are dominant, the interface is localized near the defect line. Due to the competition between energy and entropy, the interface delocalizes at the delocalization temperature T_D below the bulk critical temperature T_c (interface depinning transition). Abraham[4,6] and

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Abraham and Švrakić[7] studied a row of weakened bonds in the interior of the model. They found that the interface delocalizes if the systems on two sides of the defect have different coupling constants. The more ordered system (with the larger coupling constant) promotes its order into the less ordered system, that is, the interface delocalizes into the less ordered region. However, delocalization does not occur if systems on both sides of the defect are equally ordered, i.e., have the same coupling constants. The exact results for the phase diagram and the defect free energy for both the boundary and internal line of defects in the $d=2$ Ising model,[4-7] as well as a Monte Carlo simulation for the case of a boundary line of defects,[8] are available.

The interface delocalization also has been found in discrete and continuum versions of the planar solid-on-solid (SOS) model with one-dimensional interface.[9-14] The case with the boundary defect line has been connected with the quantum mechanical problem of a particle moving in a semi-infinite potential well, where both localized and delocalized states are possible.[9-13] The internal defect line with the same coupling constants on both sides of the defect corresponds to the problem of a symmetric potential for which only bound states exist, i.e., the interface is always bound to the defect.[9-13] The internal defect line with unequal coupling constants on two sides of the defect corresponds to the problem of a particle moving in an asymmetric, finite potential well. In this problem both localized and delocalized solutions are found.[14]

Švrakić[15] and Mihajlović and Švrakić[16] used real-space renormalization group methods[17] to study the problem of the interface delocalization in the $d=2$ Ising model. They calculated the phase diagrams and the defect free energies for the model with defect line at the boundary and for the internal line of defect bonds. The results obtained by the renormalization group method[15,16] are consistent with the exact calculations.[4-7]

Considering higher dimensional systems ($d>2$), a few results for the interface delocalization problem in the SOS and Gaussian models are known.[3,18] Burkhardt and Vieira[18] analysed the SOS and Gaussian models in higher dimensions using the mean-field theory. They found that the interface delocalizes for all dimensions $d>2$ in the SOS model, but not in the Gaussian model. Bricmont *et al.*[3] studied, using exact analysis, several problems connected with the statistical mechanics of surfaces and interfaces for the SOS, Gaussian, Blume–Capel, and Ising models. The exact analysis of the three-dimensional Ising model is mathematically complicated. There are expectations, supported by the mean-field theory[19] and heuristic arguments,[3] that the interface delocalization phenomenon also occurs in the $d=3$ Ising model.

The aim of this work is to study the interface delocalization problem in the three-dimensional Ising model using the real-space renormalization group method. We analyze delocalization of the interface for the defect plane at the boundary of the system and for the internal defect plane in the simple cubic lattice. The interface delocalization is found in the case of a boundary defect plane and in the case of an internal defect when the systems on two sides of defect plane are unequally ordered. An important question can be posed concerning the influence of the roughening transition[4,20] at temperature T_R, $0 < T_R < T_c$, on the results of this work. There are two different regimes of the interface delocalization in the $d=3$ Ising model. For $T_D > T_R$ we have continuous interface delocalization as in the $d=2$ Ising model. In the second regime, for $T_D < T_R$, we have stepwise interface delocalization. The phase diagrams obtained in this work are valid only in the continuous interface delocalization regime.

2. RENORMALIZATION GROUP FOR THE INTERFACE DELOCALIZATION

We consider the simple cubic Ising lattice of N^d spins in a zero field and with nearest neighbor ferromagnetic coupling J. It is possible to introduce periodic boundary conditions in $d-1=2$ directions and anti-periodic boundary conditions in one direction. A plane of defects with coupling $K_d = -J/k_B T$ is placed in the interior of the system. At one side of the defect plane the couplings have values $K_1 = -J_1/k_B T$, and at the other $K_2 = -J_2/k_B T$, as shown in Fig. 1. We also assume that $K_1 > K_c$ and $K_2 > K_c$, where $K_c \sim T_c^{-1}$ is the bulk critical temperature, i.e., both systems are in the ordered phase. This represents the general model for analysis of

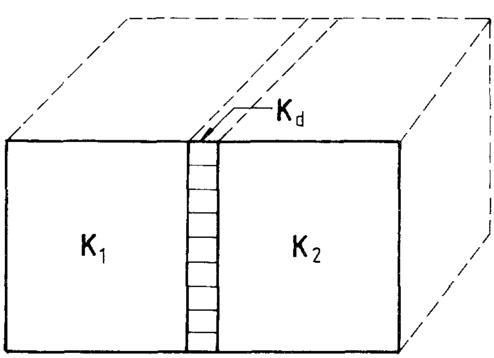

Fig. 1. The general model for analysis of interface delocalization in the three-dimensional Ising model. All horizontal couplings in the internal defect plane have values K_d. All couplings at the left side of the defect plane have values K_1, and those at the right side have values K_2.

the critical phenomena near surfaces, interfaces, and defects in the three-dimensional lattice. The case of a boundary defect plane is obtained from this model if we set $K_1 = \infty$, $K_2 < \infty$, and $K_d < K_2$. The conditions $K_1 \neq K_2$, $K_d \neq 0$ correspond to the model with an internal defect plane. Finally, for $K_d = 0$ we obtain two independent models with free surfaces. It should be noted that our model for the study of the interface delocalization in $d = 3$ is a simple generalization of its two-dimensional analog.[16] The real-space renormalization group method[17] has been used in the past for analysis of surface critical phenomena in the $d = 3$ Ising model.[21,22]

In this work we use real-space renormalization group methods to study interface delocalization in the $d = 3$ Ising model with a defect plane. We apply the first-order cumulant expansion approximation. In previous papers[15,16,23,24] this approximation has been successfully used in the analysis of different interfacial problems. In Ref. 23 we calculated the interfacial free energy of the square Ising model using several versions of cumulant, the Migdal–Kadanoff and cluster approximations to the renormalization-group equations. We introduced the interface into the system as a "seam" of defect couplings $K_d = -K$. The defect free energy is then equal to the interfacial free energy. We also gave a general analysis of problems within real-space renormalization group schemes for the calculation of defect and interfacial free energy in a hypercubic, d-dimensional Ising model. The results for the interfacial free energy obtained by the first-order cumulant expansion approximation are quantitatively consistent with the exact result in $d = 2$[23] and with the known rigorous results[4,25] in $d = 3$.[24] The same approximation also yields good quantitative results for the interface delocalization problem in the $d = 2$ Ising model.[15,16]

We find the following recursion relations for our model in $d = 3$:

$$K_j' = 4K_j \langle S(K_j) \rangle^2, \qquad j = 1, 2 \tag{1}$$

$$K_d' = 4K_d \langle S(K_1) \rangle \langle S(K_2) \rangle \tag{2}$$

where $\langle S(K_j) \rangle$ is the average value of the spin in the basic $2 \times 2 \times 2$ cell. The expression for $\langle S(K_j) \rangle$ depends on the choice of the projection rule. We use the M1 projection rule, which has been introduced in the renormalization group analysis of surface phenomena,[21,22] but is also suitable for interfacial problems.[23,24]

We first consider the model with the boundary defect plane. Here $K_1 = \infty$, $\lim_{K_1 \to \infty} \langle S(K_1) \rangle = 1$, and the recursion relations (1) and (2) become

$$K_2' = 4K_2 \langle S(K_2) \rangle^2 \tag{3}$$

$$K_d' = 4K_d \langle S(K_2) \rangle \tag{4}$$

Following Abraham's work in two dimensions,[5] we take $K_d = aK_2$, $0 \leqslant a \leqslant 1$. Relations (3) and (4) after n iterations become

$$K_2^{(n)} = 4^n K_2 \prod_{i=0}^{n-1} \langle S(K_2^{(i)}) \rangle^2 \tag{5}$$

$$K_d^{(n)} = 4^n a K_2 \prod_{i=0}^{n-1} \langle S(K_2^{(i)}) \rangle \tag{6}$$

where $K_2^{(i)}$ is the ith iterate of K_2. The couplings $K_2^{(\infty)}$ and $K_d^{(\infty)}$ are obtained from (5) and (6) after infinitely many iterations (which is in practice always less than 20). If we disregard for the moment the existence of the roughening transition temperature, we can say that two possibilities can occur: if $K_d^{(\infty)} < K_2^{(\infty)}$, the interface is localized, whereas the case $K_d^{(\infty)} > K_2^{(\infty)}$ corresponds to the delocalization of the interface. The delocalization transition temperature $T_D(a)$ for a given value of a is obtained from the condition $K_d^{(\infty)} = K_2^{(\infty)}$. Therefore, the phase boundary is given by

$$a = \prod_{i=0}^{\infty} \langle S(K_2^{(i)}) \rangle \tag{7}$$

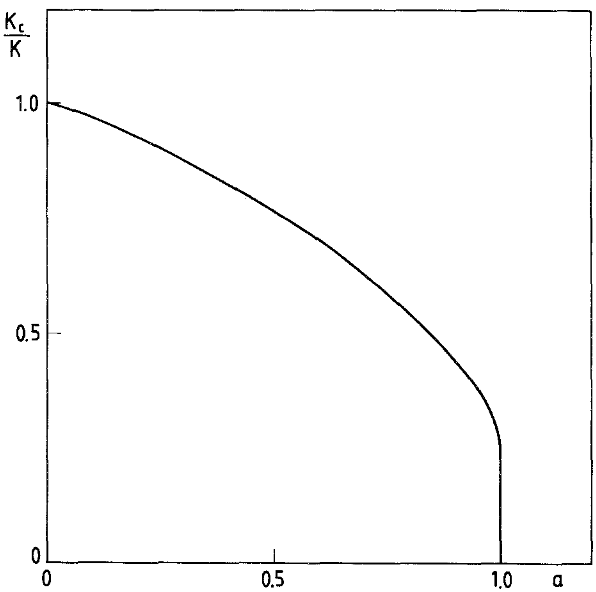

Fig. 2. Phase diagram for interface delocalization in the model with boundary defect plane. The interface is localized in the region below the curve.

As we say in the Introduction, the phase diagrams in this work are correct only in the regime of continuous interface delocalization, i.e., for $T_D > T_R$. The method and the model we analyze here cannot give stepwise interface delocalization at $T_D < T_R$. For $K_d^{(\infty)} > K_2^{(\infty)}$ and $T_D < T_R$ we can only say that the interface is not on the defect, but it can still stay near the defect. The delocalization phase diagram for the boundary defect plane obtained from (7) is shown in Fig. 2. The defect free energy is defined as[4,25]

$$F(K, K_d) = \lim_{N \to \infty} N^{-2}[\ln Z(+-) - \ln Z(++)] \tag{8}$$

where $Z(++)$ $[Z(+-)]$ is the partition function of the system with periodic (antiperiodic) boundary conditions. From (8) and the recursion relations (3) and (4) we find

$$F(K, K_d) = \lim_{i \to \infty} \left(-\frac{2K_d^{(i)}}{4^i}\right) \qquad \text{if} \quad K_d^{(i)} < K^{(i)} \tag{9}$$

and

$$F(K, K_d) = \lim_{i \to \infty} \left(-\frac{2K^{(i)}}{4^i}\right) \qquad \text{if} \quad K_d^{(i)} > K^{(i)} \tag{10}$$

The defect free energy is calculated from (9) below the delocalization transition temperature $T_D(a)$ and from (10) above $T_D(a)$. Figure 3 shows the defect free energies for the model with the boundary defect plane.

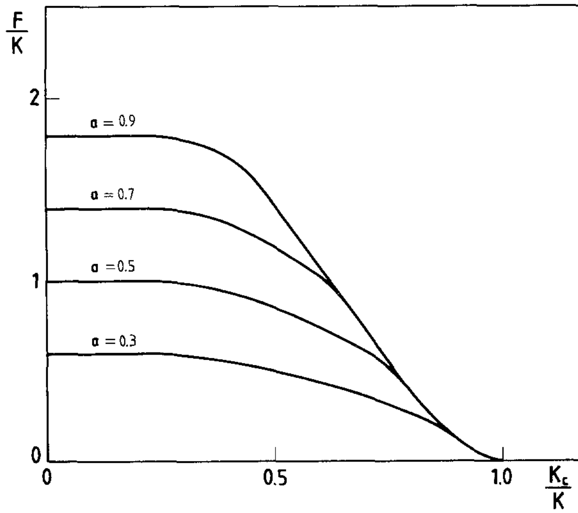

Fig. 3. Defect free energy for the model with boundary defect.

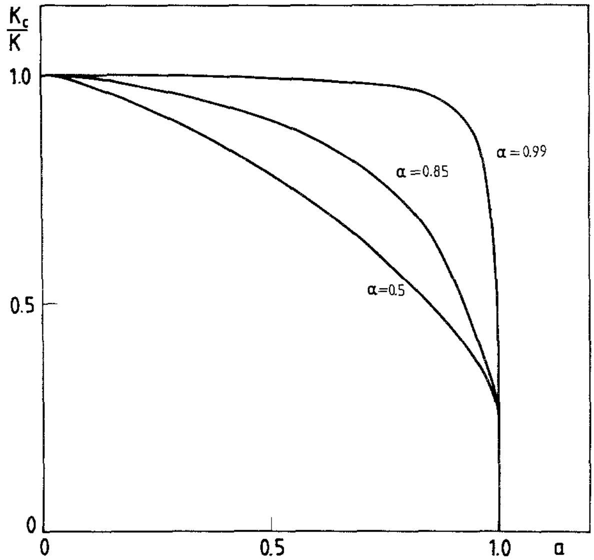

Fig. 4. Delocalization phase diagram for the model with internal defect plane obtained for various values of the parameter $\alpha = K_2/K_1$. The interface is localized in the regions below these curves. For $\alpha = 1$ $(K_2 = K_1)$ the interface is always localized.

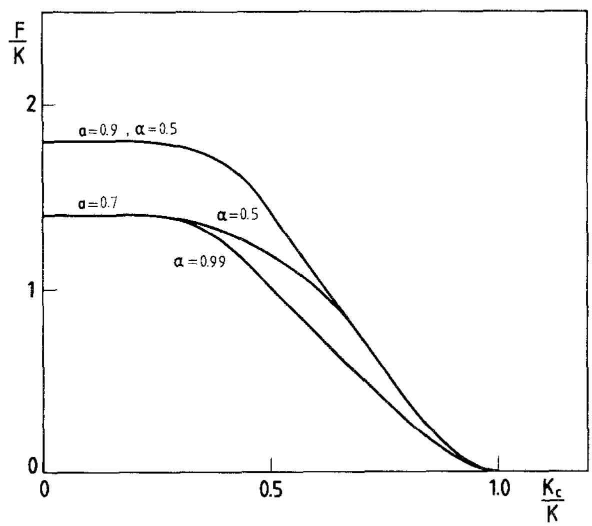

Fig. 5. Defect free energy for the model with internal defect and $\alpha \neq 1$ $(K_2 \neq K_1)$.

Now, consider the interface delocalization for the internal defect plane, i.e., $K_d < K_2 < K_1$, $K_d = aK_2$, $0 \leqslant a \leqslant 1$. By iterating the recursion relations (1) and (2) we get

$$K_j^{(n)} = 4^n K_j \prod_{i=0}^{n-1} \langle S(K_j^{(i)}) \rangle^2, \qquad j = 1, 2 \tag{11}$$

$$K_d^{(n)} = 4^n a K_2 \prod_{i=0}^{n-1} \langle S(K_1^{(i)}) \rangle \langle S(K_2^{(i)}) \rangle \tag{12}$$

The phase diagram calculated from the condition $K_d^{(\infty)} = K_2^{(\infty)}$ is given by

$$a = \left[\prod_{i=0}^{\infty} \langle S(K_2^{(i)}) \rangle \right] \Big/ \left[\prod_{i=0}^{\infty} \langle S(K_1^{(i)}) \rangle \right] \tag{13}$$

and it is shown in Fig. 4. In the same way as for Eq. (7), this phase diagram is valid only in the regime of continuous interface delocalization. Figure 5 shows the defect free energies in the case of the internal defect plane that are obtained from (9) and (10), using the recursion relations (11) and (12).

Finally, for $K_1 = K_2 = K$ and arbitrary $K_d = aK \neq 0$, the recursion relations (1) and (2) become

$$K' = 4K \langle S(K) \rangle^2 \tag{14}$$

$$K'_d = 4K_d \langle S(K) \rangle^2 = 4aK \langle S(K) \rangle^2 \tag{15}$$

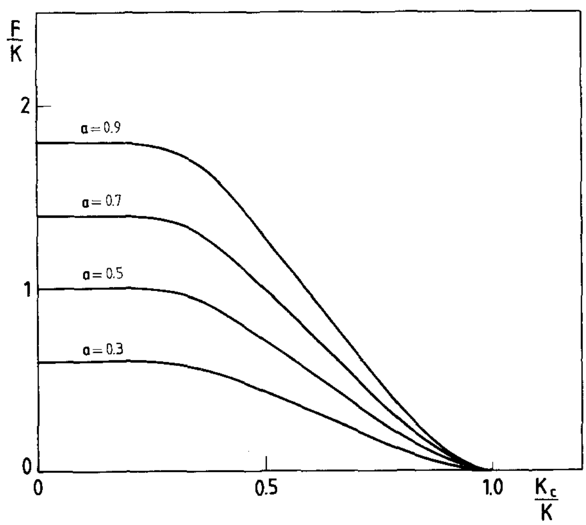

Fig. 6. Defect free energy for the model with internal defect and $\alpha = 1$ $(K_2 = K_1)$.

Because $a < 1$ is assumed, the inequality $K_d^{(n)} < K^{(n)}$ remains for arbitrarily large n, and the interface is always localized. The defect free energy in this case is calculated from (9), with (14) and (15), and the result is shown in Fig. 6.

3. CONCLUSIONS

In this work we have studied the interface delocalization in the three-dimensional Ising model for the boundary defect plane and the internal defect plane. We use the first-order cumulant expansion approximation. Our calculations confirm the expectations of the mean-field theory[19] and heuristic arguments[13] that interface delocalization occurs in the three-dimensional Ising model. Delocalization of the interface is found for the boundary defect plane and the internal defect plane between two systems with different degree of order. In the case of the internal defect plane, when coupling constants on both sides of the defect are the same, no delocalization is found, in analogy to $d = 2$ model.

ACKNOWLEDGMENTS

I am grateful to N. M. Švrakić for many discussions about the problems of real-space renormalization and interfaces and to B. Tadić for critical reading of the manuscript.

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