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Delocalization of an interface in the two-dimensional antiferromagnetic Ising model

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Abstract. It is shown that a magnetic field reduces the elasticity of an interface, and consequently enhances its delocalization in the RSOS limit of the two-dimensional antiferromagnetic Ising model with a row of weakened bonds. As pointed out, basically the same mechanism is responsible for the vanishing of the roughening temperature in the three-dimensional antiferromagnetic Ising model.

1. Introduction

One of the very intensively studied topics in statistical mechanics is interfacial behaviour (for a recent review see [1]). For discrete three-dimensional models, its characteristic phenomenon is the so-called roughening transition [2]. Up to now there has been only one exactly solvable model (BCSOS) which exhibits the roughening transition [3]. Furthermore, the roughening transition in the ferromagnetic Ising model and the corresponding solid-on-solid (SOS) model are believed to be of the same nature as the BCSOS model.

Recently we have shown that a sufficiently strong magnetic field $H > H_c$ in the three-dimensional antiferromagnetic Ising model leads to a strong degeneracy of the ground-state interface [4]. For the two-dimensional model, such degenerate configurations resemble random walk trajectories [5] while in the three-dimensional case the ground state can be regarded as a high-temperature limit of the BCSOS model. This means that the degeneracy is so strong that the interface is already rough even at the ground state [4]. However, our arguments were based only on ground-state considerations whereas it would be very desirable to study also non-zero-temperature properties of this model in the whole range of a magnetic field. Of particular importance is the change of the roughening temperature with magnetic field. It seems, however, that for the three-dimensional antiferromagnetic Ising model it might be difficult to perform Monte Carlo simulations or to adopt directly other approaches which would be able to detect the influence of a magnetic field on the roughening transition, and in particular to show its vanishing in the limit $H \to H_c$. It should be clear that the critical field H_c, which is equal to $4J$ in the three-dimensional Ising antiferromagnet, is different from the critical field $H_c^* = 6J$, at which there occurs the second-order phase transition to the paramagnetic phase (J is the nearest-neighbour interaction).

On the other hand, it is well known [1] that in two-dimensional models there is a certain analogue of the roughening transition, namely the (so-called) delocalization transition. The

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bound state of an interface is then achieved as a result of some attractive potential which can be realized, for example, as a row of weakened bonds [6]. Above a certain temperature T_D, this attractive force is not sufficient and thermal fluctuations delocalize the interface. In the RSOS limit (where the strength of vertical bonds goes to infinity and successive steps of the interface have the length of, at most, one lattice spacing), models of this phenomenon are much more tractable and it is believed that such a limit does not change the nature of the interfacial behaviour.

In the next section we study the RSOS model which mimics the interfacial behaviour in the two-dimensional antiferromagnetic Ising model in the presence of a magnetic field and an attractive potential. In the last section we extend our arguments to the three-dimensional antiferromagnetic Ising model.

2. The model and its properties

Consider the two-dimensional antiferromagnetic Ising model with boundary conditions which induce an interface. The bottom row has weakened vertical bonds and the interface is attracted to this row. In the SOS limit, in which the strength of vertical bonds goes to infinity, the interface is described by the Hamiltonian

$$\mathcal{H} = 2J\sum_{i=1}^{N-1}|n_i - n_{i+1}| + H\sum_{i=1}^{N}(-1)^{i-1}[1-(-1)^{n_i}] - U\sum_{i=1}^{N}\delta_{n_i,0}, \qquad (2.1)$$

where $n_i = 0, 1, 2, \ldots$ and $i = 1, 2, \ldots, N$ (N stands for the number of columns in our model and is assumed to be even). Hereafter, the horizontal nearest-neighbour interaction J, which can be regarded as the elasticity of the interface, is set to unity. The magnetic field H favours the configurations with even n_i for odd i and with odd n_i for even i. This can be changed, however, by modifying boundary conditions. Then the magnetic field would favour odd n_i for odd i and vice versa, but of course, physical results are the same. Such an interface adjusted to the magnetic field goes always between (++) pairs of spins [4,5]. Of course, for a finite magnetic field this effect is 'smeared' by thermal fluctuations. The pinning potential $U > 0$ favours the configurations with $n_i = 0$. A Hamiltonian similar to (2.1) for $U = 0$ and $n_i = 0, \pm1, \pm2, \ldots$ has already been studied [5]. To simplify calculations, we impose on the model (2.1) the following condition

$$|n_i - n_{i+1}| \leqslant 1 \qquad \text{for} \qquad i = 1, 2, \ldots, N-1. \qquad (2.2)$$

To study thermodynamic properties of (2.1) we have to find the free energy F defined as

$$F = -k_B T \ln Z \qquad Z = \sum_{\{n_i\}} \exp(-\beta\mathcal{H}), \qquad (2.3)$$

where $\beta = 1/k_B T$, k_B is the Boltzmann constant and T is the temperature. To calculate Z, let us define the transfer matrix $T(H)$ such that

$$T_{nm}(H) = \exp\{-\beta[2|n-m| + H(1-(-1)^n) - U\delta_{n,0}]\} \qquad (2.4)$$

where $n, m = 0, 1, 2, \ldots$. In the Hamiltonian (2.1), the contributions from the magnetic field have opposite signs for adjacent columns and thus in the thermodynamic limit $N \to \infty$, the free energy is determined by the largest eigenvalue λ_M of the product $T(H)T(-H)$

$$F = \frac{-k_B T N}{2} \ln \lambda_M \qquad (2.5)$$

This eigenvalue can be found as a solution of the following secular equation

$$\lambda\varphi_0 = \varphi_0 A(A+BC^2) + \varphi_1 AC(A+B) + \varphi_2 ABC^2 \tag{2.6}$$

$$\lambda\varphi_1 = \varphi_0 C(AB^{-1}+1) + \varphi_1(AB^{-1}C^2 + B^{-1}C^2 + 1) + \varphi_2 C(1+B^{-1}) + \varphi_3 B^{-1}C^2 \tag{2.7}$$

$$\lambda\varphi_{2n} = (\varphi_{2n-2} + \varphi_{2n+2})BC^2 + (\varphi_{2n-1} + \varphi_{2n+1})C(B+1) + \varphi_{2n}(2BC^2+1) \tag{2.8}$$

$$\lambda\varphi_{2n+1} = (\varphi_{2n-1} + \varphi_{2n+3})B^{-1}C^2 + (\varphi_{2n} + \varphi_{2n+2})C(B^{-1}+1) + \varphi_{2n+1}(2B^{-1}C^2+1) \tag{2.9}$$

where $n = 1, 2, \ldots$ and

$$A = e^{\beta U} \qquad B = e^{2\beta H} \qquad C = e^{-2\beta}. \tag{2.10}$$

The remaining part of this section is devoted to studying critical properties of the model (2.1).

2.1. *The case $H = 0$*

Although the properties of our model for $H = 0$ are well known [1], we describe them here briefly. The ground state configuration of the interface is given by

$$n_i = 0 \qquad \text{for} \qquad i = 1, 2, \ldots, N. \tag{2.11}$$

In the bound state $T < T_D$, the unnormalized eigenvector φ_n for $n = 0, 1, 2, \ldots$, which corresponds to the eigenvalue λ_M, has the form

$$\varphi_n = e^{-\mu n}. \tag{2.12}$$

The eigenvalue λ_M and the parameter μ are immediately determined from the secular equation (2.6)–(2.9), which, assuming (2.12), is equivalent to the following two equations

$$\lambda_M = e^{\beta U}(1 + e^{-\mu}e^{-2\beta}) \tag{2.13}$$

and

$$\lambda_M = 1 + 2e^{-2\beta}\cosh(\mu). \tag{2.14}$$

For $H = 0$, equations (2.8) and (2.9) as well as equations (2.6) and (2.7) are equivalent. Of particular importance for us is the parameter μ, which, determined from (2.13) and (2.14), can be written as

$$\mu = \ln\left\{\frac{1}{2}e^{2\beta}(e^{\beta U} - 1)\left[1 + \left(1 + \frac{4e^{-4\beta}}{e^{\beta U} - 1}\right)^{1/2}\right]\right\}. \tag{2.15}$$

As follows from (2.12), the critical point, which can be regarded as a delocalization transition in our model, can be determined from the condition that $\mu = 0$, or equivalently

$$e^{\beta_D^0 U}(1 + e^{-2\beta_D^0}) = 1 + 2e^{-2\beta_D^0} \tag{2.16}$$

where $\beta_D^0 = 1/k_B T_D^0$. Notice that for small U equation (2.16) leads to

$$U \sim T_D^0 e^{-2\beta_D^0}. \tag{2.17}$$

2.2. *The case* $H = +\infty$

In this case an infinitely large magnetic field suppresses unfavourable configurations at any temperature. The ground state thus has the tooth-like form

$$n_i = \begin{cases} 0 & \text{for } i = 1, 3, 5, \ldots, N-1 \\ 1 & \text{for } i = 2, 4, 6, \ldots, N. \end{cases} \tag{2.18}$$

Below T_D, the eigenvector φ_n has again the exponentially decaying form (2.12) but now *the only non-zero components correspond to even n*

$$\varphi_n = \begin{cases} e^{-\mu n} & \text{for } n = 0, 2, 4, \ldots \\ 0 & \text{for } n = 1, 3, 5, \ldots. \end{cases} \tag{2.19}$$

We find from the secular equation that μ and λ_M have to satisfy

$$\lambda_M = e^{\beta U} e^{-4\beta}(1 + e^{-2\mu}) \tag{2.20}$$

and

$$\lambda_M = 2e^{-4\beta}(\cosh(2\mu) + 1). \tag{2.21}$$

The critical temperature found from the condition $\mu = 0$ is given as

$$T_D^{\infty} = \frac{U}{\ln 2}. \tag{2.22}$$

Notice that for small U we have

$$T_D^{\infty} \ll T_D^0. \tag{2.23}$$

The reason for this inequality is clear. Elementary excitations for $H = +\infty$ require only the energy $U \ll 1$ and since U is the only energy scale in this case, the proportionality of T_D and U given in (2.22) is not surprising. On the other hand, elementary excitations for $H = 0$ require the energy of the order of unity. Competition between the entropy, the attractive potential U and the elasticity ($J = 1$) gives the relation (2.17).

In other words, we can say that for $H = +\infty$ to excite the interface we do not need to increase its length, we only have to overcome the attractive potential U.

2.3. *The case* $0 < H < +\infty$

It is simple to show that the ground state has the structure (2.11) for $H < H_c = 2 + U/2$ while for larger values of H it has the tooth-like form (2.18). Of course, for $H = 0$ and for $H = +\infty$ the eigenvectors (2.12) and (2.19), respectively, satisfy the equations (2.6)–(2.9). None of them, however, can be used as a solution of the secular equation for $0 < H < +\infty$. The structure of equations (2.8)–(2.9) suggests that the eigenvector may be chosen in the form

$$\varphi_n = \begin{cases} e^{-\mu n} & \text{for } n = 0, 2, 4, \ldots \\ q e^{-\mu n} & \text{for } n = 1, 3, 5, \ldots \end{cases} \tag{2.24}$$

with some positive parameter q. Substituting (2.24) into the secular equation (2.6)–(2.9), we obtain the following set of four equations

$$\lambda = A(A+BC^2) + qAC(A+B)e^{-\mu} + ABC^2e^{-2\mu} \tag{2.25}$$

$$\lambda q = C(AB^{-1}+1)e^{\mu} + q(AB^{-1}C^2 + B^{-1}C^2 + 1) + C(B^{-1}+1)e^{-\mu} + qB^{-1}C^2e^{-2\mu} \tag{2.26}$$

$$\lambda = 2BC^2\cosh(2\mu) + 2qC(B+1)\cosh(\mu) + 2BC^2 + 1 \tag{2.27}$$

$$\lambda q = 2qB^{-1}C^2\cosh(2\mu) + 2C(B^{-1}+1)\cosh(\mu) + q(2B^{-1}C^2+1). \tag{2.28}$$

Unfortunately, having only three parameters λ, μ, and q, we cannot satisfy these four equations. However, a reasonable approximation can be obtained if we require the fulfillment of only three of them, namely (2.25), (2.27) and (2.28). Indeed, it is easy to show that such an approximation in the limiting cases $H = 0, +\infty$ gives the exact results (2.16) and (2.22), respectively.

For arbitrary H, the critical temperature in this approximation is given as a solution of the following equation

$$r^2(B+1) + 2rC(B - B^{-1}) - B^{-1} - 1 = 0 \tag{2.29}$$

where

$$r = \frac{4BC^2 + 1 - 2ABC^2 - A^2}{C[A(A+B) - 2(B+1)]}. \tag{2.30}$$

The way to improve this zeroth-order approximation is straightforward. We can assume that the eigenvector has the form (2.24) but the coefficient φ_0 has to be determined independently, so as to satisfy the equations (2.25)–(2.28). But now the secular equation for φ_2 is not satisfied. The exponential form of the eigenvector suggests that this inconsistency is less troublesome than the one for φ_1 and that this approximation should be more accurate. In principle, it is easy to construct an nth-order approximation where the secular equation is inconsistent only for φ_{n+1}. It seems that in the limit $n \to \infty$ such a series approximation should be convergent to the exact solution. The plot of T_D as a function of H calculated using the zeroth-($\cdots\cdots$) and first-order (——) approximations for $U = 0.5$ and $U = 0.1$ shows that even the zeroth-order approximation seems to be accurate for small values of U (figure 1).

For small values of U, the critical temperature T_D changes abruptly around $H \sim H_c$. For $H > H_c$ we basically have the situation described in section 2.2, with a tooth-like ground state, tensionless interface and, consequently, low critical temperature $T_D \sim U$. On the other hand, for $H < H_c$ the elasticity of the interface considerably increases, which implies substantial raising of the critical temperature T_D. The idea that a magnetic field can be regarded as a factor which changes the elasticity of the interface is elaborated below.

2.4. Reduced elasticity approximation

As is already clear, a magnetic field favours certain configurations of an interface and suppresses others. This suggests that a reasonable approximation for the model (2.1) can be obtained by getting rid of the class of the most unfavourable configurations. As a matter of fact, the result presented in section 2.2 can be regarded as an extreme case of such an

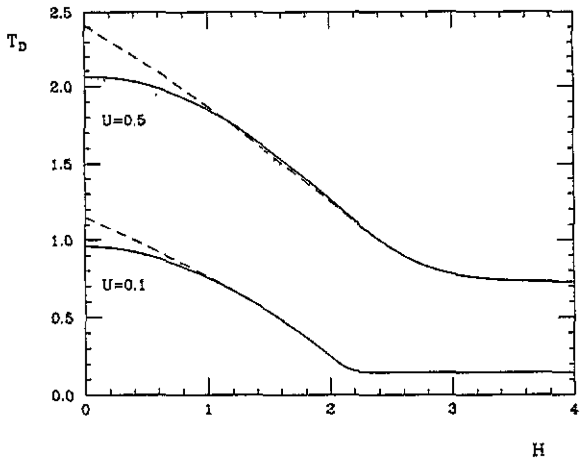

Figure 1. The critical temperature T_D as a function of the magnetic field H calculated with the use of the zero-order (2.29) (······), first-order (——), and the 'reduced elasticity' (2.34) (----) approximations. For $U = 0.1$ lines (······) and (——) nearly overlap.

approach, where the only allowed configurations have even heights at odd columns and vice versa. In fact, if we take into account the Boltzmann factor, these odd–even configurations appear to be dominant for $H \gg H_c$. However, in such a way we obtain an interface of a constant length and hence the results (e.g. the critical temperature) appear to be field-independent.

The dominance of the odd–even configurations breaks down around $H = H_c$, where other configurations provide significant contributions as well. The extended class of low-energy configurations is specified below.

Specification. For $H \sim H_c$, the representative configurations have even heights at odd columns and vice versa, with the exception that an odd height at an odd column is allowed provided that in nearest-neighbouring columns the height of the interface is the same. The analogous rule applies to even columns.

It seems plausible that that class of configurations is representative also for H slightly smaller than H_c.

For the RSOS model with the allowed configurations specified above, the secular equation has the form

$$\lambda\varphi_0 = \varphi_0(A^2 + AD^2) + \varphi_1 AD + \varphi_2 AD^2 \tag{2.31}$$

$$\lambda\varphi_{2n-1} = (\varphi_{2n-2} + \varphi_{2n})D + \varphi_{2n-1} \tag{2.32}$$

$$\lambda\varphi_{2n} = (\varphi_{2n-2} + \varphi_{2n+2})D^2 + (\varphi_{2n-1} + \varphi_{2n+1})D + \varphi_{2n}(2D^2 + 1) \tag{2.33}$$

where $n = 1, 2, \ldots$ and $D = \exp(-\beta(2 - H))$.

In the bound state, the eigenvector of (2.31)–(2.33) corresponding to the largest eigenvalue has exactly the form (2.24). After elementary calculations, the critical temperature can be found as a solution of the following equation

$$(D^2 + 1)^{1/2} = \frac{2D^2 + 1 - A^2 - AD^2}{D(A - 2)}. \tag{2.34}$$

For $U = 0.1$ and 0.5, the plot of T_D as a function of H is shown in figure 1. For $H > 1$, the approximation (2.34) (----) is in good agreement with the first-order approximation. The agreement is particularly evident for $U = 0.1$. In the limit $H \to \infty$, the formula (2.34) is equivalent to (2.22). Thus, figure 1 confirms that, indeed, the chosen class of configurations is sufficient to describe adequately the behaviour of the model (2.1) for H not much smaller than H_c (in this case for $1 < H < \infty$).

Why should we struggle to construct an approximation which is valid only in a certain range of a magnetic field while the approximations presented in section 2.3 are accurate in the whole range? The main reason stems from the fact that the approximation (2.34) has a certain physical interpretation which can be extended to higher-dimensional models as well, while it is almost impossible to apply the previous approximations to such models. The above mentioned interpretation is easy to grasp if we notice that the whole effect of a magnetic field is now incorporated in the factor D which can be seen as the exponent of the reduced elasticity

$$\bar{J} = (1 - H/2) \tag{2.35}$$

in the RSOS model defined in the specification. This can also be understood using a simple argument, which in the next section will be generalized to the three-dimensional antiferromagnetic Ising model. Neglecting the attractive potential U, which can be included separately, let us calculate the energy of a configuration of the interface which satisfies the conditions imposed in the specification. The energy ϵ is measured with respect to the flat configuration (2.11). First let us consider a single excitation of the height of unity and of an arbitrary horizontal length. According to the specification, the length must be an odd number and consequently the energy ϵ is always equal to $4 - 2H$. Excitations of larger heights can be built layer by layer, which always increases the energy by the same amount $4 - 2H$.

Thus, the resulting model is equivalent to the RSOS model with the Hamiltonian

$$\mathcal{H}' = 2\bar{J} \sum_{i=1}^{N-1} |n_i - n_{i+1}| - U \sum_{i=1}^{N} \delta_{n_i,0} \tag{2.36}$$

where the elasticity constant $\bar{J}$ is given by (2.35) and allowed configurations are described in the specification.

According to (2.35), we have $\bar{J} < 0$ for $H > 2$. This means that in the model (2.36) the favourable configurations are the 'wrinkled' ones, i.e. those of large length. Due to the attractive potential, the change of the ground state is shifted by $U/2$ and appears at $H_c = 2 + U/2$.

3. Discussion

In the previous section we have studied the RSOS model which mimics the behaviour of an interface in the two-dimensional antiferromagnetic Ising model in the presence of a magnetic field H and with an attractive potential U at the bottom row. The striking effect is the abrupt change of the critical temperature T_D for a small value of U around $H = 2$. According to the main result of section 2.4, we can regard this effect as caused by vanishing of the elasticity constant in a modified RSOS model (2.36). An accompanying effect is the change in the ground state which for $H > H_c = 2 + U/2$ has a tooth-like structure.

It seems that the influence of the magnetic field on the interfacial behaviour in the presented RSOS model (2.1) is basically similar to that in the three-dimensional antiferromagnetic Ising model. In the same way as described in section 2.4, we can argue that as H approaches $H_c = 4$ from below, the dominant excitations satisfy certain parity conditions with respect to the sum of the two coordinates S: even height for odd S and vice versa. And also as in section 2.4, the violation of these conditions is allowed provided that the nearest-neighbouring columns (now four of them) have the same height. Considering the energy ϵ of the excitations of unity-height, one finds easily that $\epsilon = p(2 - H/2)$, where p is the perimeter of the excitation (to find p, one counts only vertical parts of the interface; for configurations with one unity-height excitation in the two-dimensional model considered in the previous section, $p = 2$). Again, as excitations of arbitrary heights can be built layer by layer, their energies are proportional to their total perimeter and to the elasticity

$$\bar{J} = 1 - \frac{H}{H_c} \qquad (H_c = 4). \tag{3.1}$$

Thus, at least for H close to H_c, the interface is described by the RSOS model in which the effect of a magnetic field is incorporated only in the elasticity constant (3.1).

As there is no attractive potential in this model, this constant gives the only energy scale. Therefore, the roughening temperature should be proportional to $\bar{J}$ and hence it should vanish at H_c. The above analysis applies to the three-dimensional antiferromagnetic Ising model only in the close vicinity of the critical field $H_c = 4$, where the roughening temperature is sufficiently small to validate the RSOS approximation.

The final remark concerns the universality of the roughening transition. It is not difficult to show that for the two-dimensional RSOS model studied in the previous section the critical exponents of the delocalization transition are the same for $H = 0$ and $H = \infty$, and also for intermediate values of the magnetic field within the introduced approximations. This suggests that the magnetic field does not change the universality class of the roughening transition in the three-dimensional antiferromagnetic Ising model either. However, for a definite answer firmer arguments are needed.

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