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Surface Effects in Some Exactly Solved Three-Dimensional Ising Models

F.C. ALCARAZ

Departamento de Física, Universidade Federal de São Carlos, Caixa Postal 676, São Carlos 13560, SP, Brasil

and

S.R. SALINAS

Instituto de Física, Universidade de São Paulo, Caixa Postal 20516, 01498, São Paulo, SP, Brasil

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Abstract We consider the effect of a surface on the properties of some exactly solved Ising models in three dimensions. For an ordered surface, we show that the local magnetization per spin may decay exponentially in the bulk. The characteristic decay length is associated with the decay of the spin-spin correlations normal to the surface. In addition, we analyze the properties of the phase diagram in $T\times\Delta$ space, whet-e T is temperature and A is the enhancement factor of the surface exchange,

1. INTRODUCTION

In this paper we consider the effect of a surface on the bulk properties of some exactly solved Ising models in three dimensions. In particular, we are able to look at a case in which the surface orders while the bulk is still disordered. This problem, which is related to some interesting physical phenomena, has attracted the attention of a number of investigators[1-3]. Early mean-field calculations[4], confirmed by series expansions[ ] and Monte Carlo analyses[1], indicate that the surface magnetization decays exponentially into the bulk with a characteristic length equal to the bulk correlation lenth. We confirm this point, and perform detailed calculations for various correlation functions, in the context of the exactly solved models.

It should be mentioned that there are some exact results for the two-dimensional Ising model with modified surface exchange[5], which are in qualitative agreement with the mean-field predictions. However, in this case there can be no surface ($d=1$) ordering at finite temperatures. Our models, on the other hand, do show surface ordering but, unlike some physically more interesting cases, do not exhibit bulk ordering.

The three-dimensional models studied in this paper are defined on a semi-infinite cubic lattice bounded by a two-dimensional surface on the $z=1$ plane. In section 2 we consider an Ising square lattice on the surface with a set of independent Ising chains along the positive z direction. This is probably the simplest case where there may occur surface ordering with a disordered bulk, The exponential decay of the surface magnetization is already present in this simple model. In section 3 we consider a square lattice Ising model, with exchange interactions $J_S = J(1+\Delta)$, on the $z=1$ plane, and a structure of four-spin interactions, with exchange $J_B = J$, on the x-z and y-z planes. In this more complex case, although the global symmetry is not broken, the planar symmetry[6] of the bulk may be spontaneously broken. This gives rise to an interesting phase diagram in T-Δ phase space. In the appendix, we introduce a simple one-dimensional Ising model, with a field applied in the first site, which shows some of the phenomena discussed in the context of the three-dimensional models.

2. SURFACE WITH CHAIN-LIKE BULK

Let us consider a square Ising lattice, on the $z=1$ plane, with nearest-neighbor exchange interactions J_S, and a set of independent Ising chains, with nearest-neighbor interactions $J_{B'}$ along the positive z direction. We then have the hamiltonian

$$H = - J_S \sum_{i,j} \sigma_{i,j,1} (\sigma_{i+1,j,1} + \sigma_{i,j+1,1})$$

$$- J_B \sum_{i,j} \sum_k \sigma_{i,j,k} \sigma_{i,j,k+1} , \qquad (2.1)$$

where $\sigma_{i,j,k} = \pm 1$, and i, j, and k, are positive integers running from 1 to N. If we assume free boundary conditions along the z direction, it is possible to write the one-to-one σ-τ transformations[7],

$$\sigma_{i,j,1} = \tau_{i,j,1}$$

$$\sigma_{i,j,2} = \tau_{i,j,1}\ \tau_{i,j,2} \tag{2.2}$$

$$\sigma_{i,j,3} = \tau_{i,j,1}\ \tau_{i,j,2}\ \tau_{i,j,3}$$

$$\cdots\cdots\cdots\cdots\cdots$$

where $\tau_{i,j,k} = \pm 1$ for all i,j,k. The transformed hamiltonian is written as

$$H' = - J_S \sum_{i,j} \tau_{i,j,1}\ (\tau_{i+1,j,1} + \tau_{i,j+1,1}) - \tag{2.3}$$

$$- J_B \sum_{i,j} \sum_k \tau_{i,j,k+1}$$

The partition function is then given by

$$Z = \mathrm{Tr}\ \exp(-\beta H) = Z_I(\beta J_S)(2 \cosh \beta J_B)^{N^3} \quad , \tag{2.4}$$

where $\beta = (k_B T)^{-1}$, k_B is Boltzmann's constant, and Z_I is the partition function of a square Ising lattice with N^2 spins. In the thermodynamic limit we have the free energy

$$f = - k_B T \lim_{N\to\infty} \frac{1}{N^3} \log Z = - k_B T \log\left[2 \cosh \beta J_B\right] \quad , \tag{2.5}$$

from which we see, as expected, that the surface plays no role on the global thermodynamic properties of this model. It should be remarked that, from eqs. (2.4) and (2.5), we can easily obtain an expression for the surface free energy, f_S. If we write $F = -k_B T \log Z$, f_S is given by

$$f_S \equiv \lim_{N\to\infty} \frac{F-N^3 f}{N^2} = \lim_{N\to\infty} \frac{-k_B\ T \log Z_I(\beta J_S)}{N^2} \quad . \tag{2.6}$$

It is then clear that f_S is the free energy per spin of the Ising square lattice on the surface.

The local magnetization is given by

$$\langle\sigma_{i,j,k}\rangle = \frac{1}{Z}\,\mathrm{Tr}\,\sigma_{i,j,k}\,e^{-\beta H} = m_I(\beta J_S)\,(\tanh\beta J_B)^{k-1}\,, \qquad (2.7)$$

for $i,j,k \geq 1$, where m_I is the spontaneous spin magnetization of the Ising square lattice. From eq, (2,7), we notice that $\langle\sigma_{i,j,k}\rangle$ vanishes identically above the critical temperature of the Ising surface, that is, for $\beta J_S < \frac{1}{2}\log(1+\sqrt{2})$. In addition to this, we have the global spontaneous magnetization

$$m = \lim_{N\to\infty}\frac{1}{N^3}\sum_{i,j,k}\langle\sigma_{i,j,k}\rangle =$$

$$= m_I(\beta J_S)\lim_{N\to\infty}\frac{1}{N}\sum_{k=1}(\tanh\beta J_B)^{k-1} = 0\,, \qquad (2.8)$$

for all temperatures.

Below the surface critical temperature it is interesting to write eq. (2.7) in the form

$$\langle\sigma_{i,j,k}\rangle = \frac{m_I(\beta J_S)}{\tanh\beta J_B}\exp\left(-\frac{k}{\xi}\right)\,, \qquad (2.9)$$

with the characteristic decay length

$$\xi = \frac{1}{|\log\tanh\beta J_B|} \qquad (2.10)$$

Further, it is easy to show that

$$\langle\sigma_{i,j,k}\,\sigma_{i,j,k+\ell}\rangle = (\tanh\beta J_B)^{\ell} \qquad (2.11)$$

from which we see that the spin-spin correlations along the chains decay with the characteristic length ξ, given by eq. (2.10).

3. SURFACE WITH PLAQUETTE INTERACTIONS

As another example, let us 'consider a square lattice Ising model, with exchange interactions J_S, on the $z = 1$ plane, and a set of four-spin plaquette interactions on the x-z and y-z planes of a cubic lattice. In this case, the bulk is still disordered at all temperatures although it presents a singular behaviour. The corresponding Ising spin hamiltonian is then given by

$$H = H_{\text{surface}} + H_{\text{bulk}} \,, \tag{3.1}$$

where

$$H_{\text{surface}} = - J_S \sum_{i,j} \sigma_{i,j,1} \left(\sigma_{i+1,j,1} + \sigma_{i,j+1,1}\right) \,, \tag{3.2}$$

and

$$H_{\text{bulk}} = - J_B \sum_{i,j,k} \left[\sigma_{i,j,k} \; \sigma_{i+1,j,k} \; \sigma_{i,j,k+1} \; \sigma_{i+1,j,k+1} \; + \right.$$

$$\left. + \; \sigma_{i,j,k} \; \sigma_{i,j+1,k} \; \sigma_{i,j,k+1} \; \sigma_{i,j+1,k+1}\right] \,, \tag{3.3}$$

where i,j,k are integers running from 1 to N.

It should be noticed that the hamiltonian (3.1) has a global symmetry, $\sigma_{i,j,k} \rightarrow -\sigma_{i,j,k}$ for all i,j,k, and a planar symmetry[6], $\sigma_{i,j,k} \rightarrow -\sigma_{i,j,k}$ for all i,j, with fixed k. Both symmetries are non-local and may in principle be spontaneously broken. However, the global symmetry is a sub-symmetry of the planar symmetry. Therefore, if the planar symmetry is not broken, the global symmetry will not be broken either. On the other hand, as we shall see in the following, the planar symmetry may be spontaneously broken without producing a bulk spontaneous magnetization. From this point of view, unlike in the case of a bona-fide three-dimensional model, the bulk effects of this example are essentially governed by two-dimensional mechanisms.

If we assume free boundary conditions along the z direction, it is possible to use the σ-τ transformations of the previous section to write the transformed hamiltonians,

$$H'_{\text{surface}} = - J_S \sum_{i,j} \tau_{i,j,1} \left[\tau_{i+1,j,1} + \tau_{i,j+1,1}\right] \,, \tag{3.4}$$

and

$$H'_{bulk} = - J_B \sum_k \sum_{i,j} \tau_{i,j,k+1} [\tau_{i+1,j,k+1} + \tau_{i,j+1,k+1}] \quad . \tag{3.5}$$

The partition function is then given by

$$Z = Z_I(\beta J_S) \, [Z_I(\beta J_B)]^N \quad , \tag{3.6}$$

where Z_I is the partition function of an Ising square lattice with N^2 sites. In the thermodynamic limit, as $\log Z_I \sim N^2$, we have the free energy per spin

$$f = - k_B T \lim_{N\to\infty} \frac{1}{N^3} \log Z \sim - \frac{k_B T}{N^2} \log Z_I(\beta J_B) \quad . \tag{3.7}$$

As expected, the thermodynamic behaviour is governed by the bulk partof the hamiltonian.

It is easy to show that the local spin magnetization is given by

$$<\sigma_{i,j,k}> = m_I(\beta J_S) \, [m_I(\beta J_B)]^{k-1} \tag{3.8}$$

for $k \geqq 1$, where m_I is the spin magnetization of the Ising square lattice, As $|m_I| < 1$, we have the global magnetization per spin

$$m = \lim_{N\to\infty} \frac{1}{N^3} \sum_{i,j,k} <\sigma_{i,j,k}> = 0 \quad , \tag{3.9}$$

which indiçates that the bulk does not order, that is, the global symmetry is not spontaneously broken. It is interesting to note that the decay effects in the bulk will occur for βJ_S, $\beta J_B > \frac{1}{2} \log(1 + \sqrt{2})$. Thus, if $\beta J_B > \beta J_S$, the surface may order without producing any bulk effects.

Let us use the σ-τ transformation to look at some correlation functions:

(i) Along a z axis we have

$$<\sigma_{i,j,k} \, \sigma_{i,j,k+\ell}> = [m_I(\beta J_B)]^{\ell} \quad , \tag{3.10}$$

for $\ell \geq 1$. From eqs. (3.8) and (3.10) we see that, as in the previous example, the local magnetization and the spin-spin correlations along a chain decay with the same characteristic length

$$\xi = \frac{1}{|\log m_I(\beta J_B)|} \tag{3.11}$$

(ii) The general two-body correlation function will be given by

$$<\sigma_{i,j,k}\,\sigma_{i',j',k+\ell}> =$$

$$= C_I(|i-i'|,|j-j'|;\beta J_S)\left[C_I(|i-i'|,|j-j'|;\beta J_B)\right]^{k-1}\left[m_I(\beta J_B)\right]^{\ell}, \tag{3.12}$$

for k,R $\geq$ 1, where $C_I(|x|,|y|;\beta J)$ is the spin-spin correlation function for a square Ising lattice, with exchange J, at a temperature $T = 1/k_B\beta$, where the spins are at distances $|x|$, $|y|$ apart, respectively along the x,y directions. Of course, if $i = i'$, and $j = j'$, we regain eq. (3.10).

(iii) The planar two-body correlation functions are given by

$$<\sigma_{i,j,k}\,\sigma_{i',j',k}> = C_I(|i'-i|,|j'-j|;\beta J_S)\left[C_I(|i'-i|,|j'-j|;\beta J_B)\right]^{\ell-1}, \tag{3.13}$$

for $k \geq 1$.

(iv) The four-body correlation functions are given by

$$<\sigma_{i,j,k}\,\sigma_{i,j,k+\ell}\,\sigma_{i',j',k}\,\sigma_{i',j',k+\ell}> = \left[C_I(|i'-i|,|j'-j|;\beta J_B)\right]^{\ell}, \tag{3.14}$$

for $\ell \geq 1$.

If we write $J_B = J$ and $J_S = J(1+\Delta)$, where Δ plays the role of an enhancement parameter, it is interesting to draw the $T\times\Delta$ phase diagram of fig. 1. Region I is strictly disordered, since there is no surface ordering and no decay effects of the local magnetization are present in the bulk. In region II the surface orders but the local magnetization in the bulk still vanishes. Finally, in region III the surface

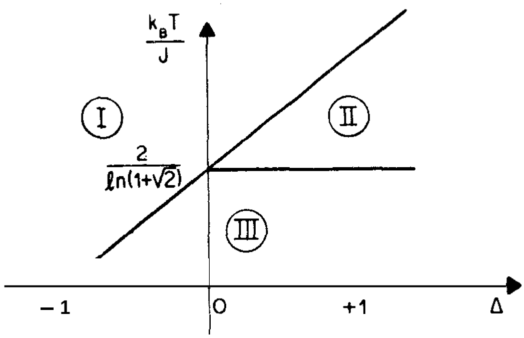

Fig.1 - The global symmetry is present in all regions of this phase diagram. In region I the surface is disordered. In region II the surface is ordered, but there are no bulk effects. In region III the surface is ordered and the local magnetization decays exponentially in the bulk. In region I, for $k_BT/J<2/\ln(1+\sqrt{2})$, the planar symmetry of the bulk spontaneously broken, although there is no ordering.

orders, and the local magnetization decays exponentially in the bulk.

It is also interesting to analyze the $T\times\Delta$ phase diagram on the basis of the decay of the correlation functions. In region II, for example, as $m_1(\beta J_B) = 0$, there are no correlations along the z direction. However, region I is much more complicated. In this region, for $k_BT/J < 2/\log(1+\sqrt{2})$, the bulk shows planar ordering, and there are spin -spin correlations along the z direction even without surface ordering. It should be pointed out that the decay of the correlations is closely connected with the breaking of the planar symmetries. In region II the planar symmetry is broken at the surface only. In region III the planar symmetry is always broken, In region I, however, there are two possibilities: (i) for $k_BT/J > 2/\log(1+\sqrt{2})$, the planar symetry is present; (ii) otherwise, the planar symmetry is broken in the bulk only.

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APPENDIX - ONE-DIMENSIONAL MODEL

One can conceive a one-dimensional model presenting decay effects of the local magnetization, in analogy with the previous three-

-dimensional examples. Let us consider the Ising hamiltonian

$$H = - h\,\sigma_1 - J \sum_{i=1}^{N} \sigma_i\,\sigma_{i+1} \ , \qquad (A.1)$$

where $\sigma_i = \pm 1$, for all i, and h is a field applied on the first spin. Using the O-T transformation, it is easy to write the partition function

$$Z = 2 \cosh \beta h (2 \cosh \beta J)^N \ , \qquad (A.2)$$

from which we have the free energy

$$f = -k_B T \lim_{N\to\infty} \frac{1}{N} \log Z = - k_B T \log\left[2 \cosh \beta J\right] \ , \qquad (A.3)$$

From this equation we see that the boundary is not relevanttodetermine the bulk thermodynamic properties.

The local magnetization is given by

$$\langle\sigma_k\rangle = (\tanh \beta h)(\tanh \beta J)^{k-1} \ , \qquad (A.4)$$

for $k \geqq 1$. It is interesting to write this expression in the form

$$\langle\sigma_k\rangle = \frac{\tanh \beta h}{\tanh \beta J} \exp\left(- \frac{k}{\xi}\right) \ , \qquad (A.5)$$

with the decay length

$$\xi = \frac{1}{|\log \tanh \beta J|} \qquad (A.6)$$

On the other hand, the spin-spin correlations are given by

$$\langle\sigma_j\, \sigma_{j+k}\rangle = (\tanh \beta J)^k = \exp\left(- \frac{k}{\xi}\right) \ , \qquad (A.7)$$

for $k \geqq 1$. Thus, as in the previous examples, the local spin magnetization decays in the bulk with the same characteristic lenth as the spin-spin correlations. Also, we have

$$m = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} <\sigma_k> \equiv 0 \quad , \qquad (A.8)$$

which confirms that the one-dimensional model does not order.

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Resumo

Consideramos o efeito de uma superfície sobre as propriedades de alguns modelos de Ising tridimensionais exatamente solúveis. No caso de uma superfície ordenada, mostramos que a magnetização local por spin pode decair exponencialmente no interior do sistema. O comprimento característico do decaimento está associado com o decaimento das correlações spin-spin normais à superfície. Também analisamos as propriedades do diagrama de fases no espaço T × Δ, onde T é a temperatura e Δ é o fator multiplicativo do parâmetro de troca da superfície.