RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 30, NUMBER 11 1 DECEMBER 1984

Surface magnetization in inhomogeneous two-dimensional Ising lattices

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(Received 20 September 1984)

A simple exact expression for the surface magnetization in the Hamiltonian limit is used to discuss the effects of slowly varying coupling constants.

Planar Ising models with a free surface and with couplings which vary with the distance from that surface have been the topic of several recent papers.[1-4] In these studies, a dependence of the form

$$K(n)=K(1+an^{-y}), \quad n \geq 1 \tag{1}$$

was assumed for at least one of the couplings, where n labels the bonds, starting from the surface, and a,y are free parameters. The couplings, therefore, approach their bulk value with a power law. Investigated were the spin correlations in the surface (exponent $\eta_{\parallel}$) and the surface magnetization m_s (exponent β_s). It was found that for $y>1$, the critical behavior is not modified, but at $y=1$ it is, and the exponents $\eta_{\parallel}$ and β_s then become continuous functions of the parameter a. Moreover, for $y=1$ and $a>a_c$, as well as for $y<1$ and $a>0$, the tendency towards order is so much enhanced near the surface that m_s does not vanish as the bulk critical temperature is approached from below.

It was shown by Burkhardt[5,6] and Cordery[7] how such a critical behavior can be understood from a renormalization-group analysis. However, for the Ising model one would also like to have a more direct explanation. The existing calculations are based either on an ingenious application of the star-triangle transformation[1-3] or on Pfaffian techniques.[4] The drawback is that both are quite involved so that the mechanism of the effects is not very transparent. In the present Rapid Communication I want to show that the surface magnetization can be obtained in a much simpler way. The mathematical origin of the unusual behavior is then clearly visible. The system which I consider is a square lattice in the Hamiltonian limit.

Let $K_1=\beta J_1$ and $K_2(n)=\beta J_2(n)$ be the vertical and horizontal couplings, respectively. The row-to-row transfer matrix in the limit of large K_1 and small $K_2(n)$ is given by $V=\exp(-K_1^*\mathcal{H})$, where K_1^* is the dual coupling of K_1 and $\mathcal{H}$ is the transverse Ising Hamiltonian[8]

$$\mathcal{H}=-\sum_{n\geq 1}\sigma_n^z-\sum_{n\geq 1}\lambda_n\sigma_n^x\sigma_{n+1}^x \ , \tag{2}$$

with $\lambda_n=K_2(n)/K_1^*$ and Pauli matrices σ_n^x, σ_n^z. Assuming the n dependence of Eq. (1), we have $\lambda_n=\lambda(1+an^{-y})$. The bulk parameter λ measures the temperature, with $\lambda>1$ corresponding to $T<T_c$. The surface magnetization can be obtained from the large distance limit of the spin-correlation function in the surface. This leads to the expression[8]

$$m_s=\langle 1|\sigma_1^x|0\rangle \ , \tag{3}$$

where $|0\rangle$ is the ground state of $\mathcal{H}$ and $|1\rangle$ is the state which, for a horizontally infinite system ($1\leq n<\infty$), becomes degenerate with $|0\rangle$ (for $\lambda>1$). The way how this degeneracy occurs, is well known from the homogeneous case $a=0$:[9,10] One diagonalizes with the help of Fermi operators, obtaining $\mathcal{H}=\sum_p \epsilon_p\alpha_p^\dagger\alpha_p+\text{const}$, where the single-particle energies ϵ_p follow from a matrix equation of the form

$$(A-B)(A+B)\phi_p=\epsilon_p^2\phi_p \tag{4}$$

in the notation of Ref. 9. It is then found that one state, which I shall call s, has exponentially small energy $\epsilon_s\sim\lambda^{-N}$ in a finite system ($n\leq N$) and a wave function $\phi_s(n)$ which is localized in a region $n\lesssim(\ln\lambda)^{-1}$ near the surface. Therefore, the state $|0\rangle$ is the vacuum of the Fermi operators α_p, and $|1\rangle=\alpha_s^\dagger|0\rangle$ has one fermion in state s. Upon expressing σ_1^x in terms of the α_p, one finds that

$$m_s=\phi_s(1) \tag{5}$$

so that the surface magnetization is completely determined by the amplitude of the state s at site 1.

The point now is that in the infinite system with $\epsilon_s=0$ the function ϕ_s can be determined from the simpler equation $(A+B)\phi_s=0$ (Ref. 11), where

$$(A+B)=2\begin{pmatrix} 1 & \lambda_1 & & & & \\ & 1 & \lambda_2 & & & \\ & & 1 & \lambda_3 & & \\ & & & \cdots & & \\ & & & & \cdots & \\ & & & & & \cdots \end{pmatrix} . \tag{6}$$

This gives a recurrence relation for $\phi_s(n)$ which can be solved explicitly for *arbitrary* values of λ_n. For the specific choice made above, it gives, setting $\phi_s(1)=C/\lambda$,

$$\phi_s(n)=C(-1)^{n+1}\lambda^{-n}\left[\prod_{k=1}^{n-1}\left(1+\frac{a}{k^y}\right)\right]^{-1} . \tag{7}$$

The constant C has to be calculated from the normalization condition $\sum_n\phi_s(n)^2=1$. In this way the spatial variation of ϕ_s determines the value of m_s. In particular, m_s is only nonzero as long as ϕ_s remains normalizable.

The various possible cases can now be discussed. In the homogeneous system ($a=0$), ϕ_s is a simple exponential function and C is readily evaluated, leading to[10] $m_s=(1-\lambda^{-2})^{1/2}$ and, hence, $\beta_s=\frac{1}{2}$. For $a\neq 0$, the simple exponential decay is modified by the product in Eq. (7). For enhanced couplings ($a>0$), ϕ_s decreases faster, at least initially. For weakened couplings ($a<0$) it decreases slower and can even increase initially. This happens if couplings near the surface become undercritical ($\lambda_n<1$). In the case $y>1$, the product converges and the form of ϕ_s is unchanged for large n. Since m_s is determined by the large

n behavior of ϕ_s for $\lambda \gtrsim 1$, its critical behavior is not modified. The case $y=1$, however, is different. The product can then be expressed in terms of gamma functions

$$\prod_{k=1}^{n-1}\left[1+\frac{a}{k}\right]=\frac{\Gamma(n+a)}{a\Gamma(a)\Gamma(n)} \tag{8}$$

and varies as n^a for $n \to \infty$. The wave function ϕ_s, therefore, varies as a power law in the region $1 << n \lesssim (\ln\lambda)^{-1}$ for $\lambda \to 1$. It is this behavior which leads to a continuously varying exponent β_s. Explicitly, one finds for $\lambda \gtrsim 1$,

$$m_s \sim \left(\int_0^\infty dn\, n^{-2a}\lambda^{-2n}\right)^{-1/2}, \tag{9}$$

so that $\beta_s=\frac{1}{2}-a$. This agrees with the result of Ref. 4 in the present limit of small couplings K_2. Actually, this formula applies only for $a<0.5$. For $a>0.5$, the function ϕ_s is modified so much that it remains normalizable even for $\lambda=1$ and, therefore, m_s stays finite at the critical temperature. In this case, one can ask how m_s approaches this finite limit and finds a power law with exponent $\beta_s'=2a-1$, which is again in agreement with Ref. 4. A complete picture is then obtained by calculating m_s for all temperatures numerically. The result for $y=1$ and various values of a is shown in Fig. 1. As one would expect, a large value of β_s means that the whole magnetization curve rises only slowly as the temperature is lowered.

The case $y<1$, finally, is again different. Here, the product in Eq. (7) varies as $\exp(an^{1-y})$ for large n. This gives a localized wave function and, therefore, a finite value of $m_s(T_c)$ for all $a>0$. It can be shown that $m_s(T_c)$ varies as a^z for small a, where $z=\frac{1}{2}(1-y)^{-1}$. The exponent β_s', which describes the approach towards this limit, turns out to be $\beta_s'=1$ here. For $a<0$, the function ϕ_s is strongly shifted away from the surface and increases exponentially in the region of subcritical couplings $n \lesssim \epsilon^{-1/y}$, where $\epsilon=1-1/\lambda$. Therefore, m_s is very small near the critical temperature, varying as

$$m_s \sim \exp(-g/\epsilon^{(1-y)/y}), \tag{10}$$

where g depends on a and y. This is the same type of anomalous critical behavior as found for the spin-correlation function at T_c.[3]

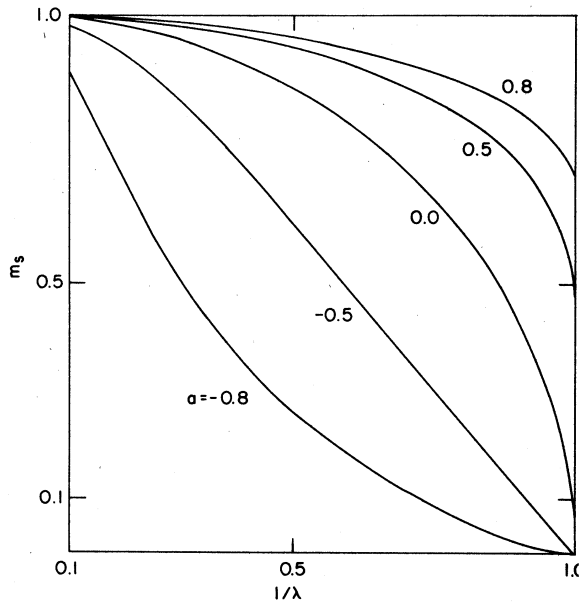

FIG. 1. Surface magnetization vs temperature (measured by λ) for $y=1$ and various values of a.

In conclusion, I have shown how the features of the surface magnetization in the case of slowly varying couplings follow from the properties of the surface state which one encounters in the transfer matrix. The case where the couplings K_1 and K_2 vary in space can be treated in the same way. A calculation of the spin-correlation function would be more difficult, since there all fermion states come into play.

I would like to thank Dr. V. J. Emery and the Brookhaven National Laboratory for their hospitality. I also thank Dr. H. Blöte for a discussion of his work. Research supported by the Division of Materials Sciences, U.S. Department of Energy under Contract No. DE-AC-76CH00016.

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[11]Equation (4) actually arises from the combination of the two matrix equations $(A+B)\phi_p=\epsilon_p\psi_p$ and $(A-B)\psi_p=\epsilon_p\phi_p$, see Ref. 9.