Real-space renormalization-group calculation for the surface tension for the triangular Ising model

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Using a modified version of the clusters we proposed recently for the real-space renormalization group, we calculate the surface tension for the Ising model on a triangular lattice. The results are in good agreement with the exact answers.

There has been much interest in studying surface tension, since the understanding of the structure of the interface separating two phases is crucial in understanding phase equilibria. Although it is very difficult to calculate the surface tension, or the interfacial free energy, from the first principles of statistical mechanics, however, various recent renormalization-group (RG) calculations seem to indicate a simple approach for calculating the approximate surface tension of an Ising ferromagnet or lattice gas.

Oliveira *et al.*[1] have employed a cell-type real-space RG transformation[2,3] and obtained results in fair agreement with the exact curve for the Ising model on a square lattice and reasonable results for three-dimensional Ising models. A more recent calculation of Curado *et al.*[4] has adapted the real-space RG developed by Reynolds *et al.*[5] (RKS) to study the longitudinal surface tension for the Ising ferromagnet on a square lattice. Although they have obtained good results, however, even with a complicated cluster having 41 bonds (corresponding to $b=5$, with b indicating the cluster size), their results are still far from convergence to the exact curve. Nevertheless, they have used some extrapolation procedures to improve their results so as to be able to compare with the exact curve. The problem of convergence of their results for the surface tension is a consequence of the slow convergence of the critical exponent ν corresponding to the correlation length calculated using the clusters of RKS. It is shown by Widom[6] based on scaling arguments that for two-dimensional lattices, the critical exponent μ corresponding to the surface tension is equal to that corresponding to the correlation length. Therefore, the exact values for μ and ν are both equal to unity as is calculated by Onsager[7] for two-dimensional lattices. Using the real-space RG approach, Curado *et al.*[4] have also shown that $\mu=\nu$ for two-dimensional systems. However, while using the $b=5$ cluster of RKS, they have obtained $\mu=\nu=1.08791$ having an error of about 8.8% comparing with the exact values. Therefore, although the use of RKS clusters leads to exact critical point,[4] nevertheless, it gives large errors for critical behavior for small b cases.

Recently, Chao[8,9] has extended the RKS approach to the triangular lattice using a three-bond cluster as the elementary cluster. Two types of clusters are constructed, which are referred to as the diagonal and longitudinal clusters.[10] The diagonal clusters give results for ν having 25 and 21% error compared with the exact value for the $b=2$ and 3 case, respectively.[8] However, the longitudinal clusters give surprisingly good results: even the simplest $b=2$ cluster leads to a value for ν, and therefore μ, with only 3.2% error[9] comparing with the exact values. We thus expect to obtain good results for the surface tension by using the longitudinal triangular clusters.

We consider an Ising ferromagnet in which a system of spins occupies the sites of a triangular lattice and interacts via nearest-neighbor couplings of strength J. The surface tension is produced when a row of antiferromagnetic interactions (the "seam") of strength $-J$ is introduced and an interface created in the uniform lattice. The resulting incremental free energy yields the surface tension. It is convenient to represent the interaction between a pair of sites by a bond having a transmissivity defined as

$$t=\tanh(J/k_BT) \ , \tag{1}$$

with k_B the Boltzmann constant and T the temperature. The situation is shown in Fig. 1, where each solid line represents a ferromagnetic bond having positive transmissivity t and each dashed line repre-

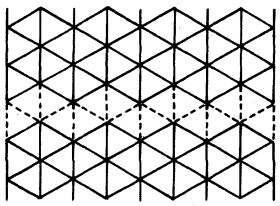

FIG. 1. The Ising ferromagnet on a triangular lattice with a row of antiferromagnetic interactions as indicated by dashed lines.

sents an antiferromagnetic bond having negative transmissivity $-t$.

Within the real-space RG approach, we then divide the lattice shown in Fig. 1 into cells having the shape of the longitudinal triangular clusters as proposed by Chao.[9] However, the cells near the seam should be represented by clusters having some ferromagnetic bonds replaced by antiferromagnetic ones. Thus, we should consider three types of clusters as shown in Fig. 2 for both the $b=1$ and 2 cases. Each $b=2$ cluster in Fig. 2 should be renormalized into one corresponding elementary cluster ($b=1$), such that the RG transformation preserves the lattice and the seam.

The first type of clusters, with all positive transmissivities, have equivalent transmissivities as given before[9]

$$R_1(t')=t' \tag{2}$$

and

$$R_2(t)=\frac{t^2(2t^4-t^3+7t^2-3t+3)}{3t^6-t^5+4t^4-t^3+4t^2-2t+1} \ . \tag{3}$$

Both the other two types of clusters with $b=1$ can be reduced to a graph with one antiferromagnetic bond for the direction of traverse indicated in Fig. 2. Thus, they have the equivalent transmissivity

$$G_1(t')=-R_1(t')=-t' \ . \tag{4}$$

The $b=2$ clusters are represented by graphs (also shown in Fig. 2) when they are to be traversed from the bottom to the top in correspondence with the way the $b=1$ clusters are traversed. To calculate the equivalent transmissivities for these graphs, we apply

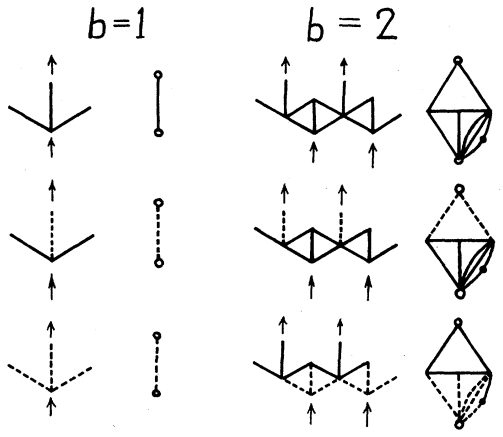

FIG. 2. Three lowest-order longitudinal triangular clusters and their corresponding graphs used for calculating the longitudinal surface tension for the Ising model on a triangular lattice. Each solid bond is to be associated with a positive transmissivity t and each dashed bond a negative transmissivity $-t$. The arrows indicate the direction of traverse.

the break-collapse method.[11] It is then easy, although rather tedious, to show that

$$G_2(t)=-R_2(t), \tag{5}$$

for both graphs containing negative transmissivities. Therefore, all three types of clusters lead to the same RG equation

$$R_1(t')=R_2(t) \ , \tag{6}$$

which, using Eqs. (2) and (3), can be written as

$$t'=\frac{t^2(2t^4-t^3+7t^2-3t+3)}{3t^6-t^5+4t^4-t^3+4t^2-2t+1} \ . \tag{7}$$

Equation (7) is the same as was obtained previously,[9] and has the fixed point $t^*=0.2801$ or $k_BT^*/J=3.475$. The correlation length critical exponent ν, as can be calculated through the equation[12]

$$\nu=\ln 2 \Big/ \ln\left[\frac{dR_2(t)}{dt} \Big/ \frac{dR_1(t)}{dt}\right]_{t^*} \ , \tag{8}$$

also has the same value ($\nu=1.032$) as was obtained previously.[9]

In order to calculate the surface tension for the Ising model, we still need a RG equation for the surface tension. Such an equation has been given by Oliveira *et al.*,[1] who have argued that since the RG transformation preserves the correlation function, and leaves the value of the partition function unchanged, therefore, along a RG trajectory

$$\xi^{d-1}f=\text{const} \ , \tag{9}$$

where f is the normalized interfacial contribution to the dimensionless free energy. Now, since the surface tension is given by

$$\gamma=-k_BTf \ , \tag{10}$$

with the lattice constant taken as unity. Thus, we obtain from (9) and (10) the following RG equation[4]:

$$(b')^{d-1}\frac{\gamma'}{T'}=b^{d-1}\frac{\gamma}{T} \ . \tag{11}$$

For the two-dimensional case, we have

$$\gamma'=\frac{b}{b'}\frac{T'}{T}\gamma \ , \tag{12}$$

where $b/b'=2$ for the case we are interested.

Equations (1), (7), and (12) enable us to obtain the flow diagram in the $\gamma-T$ space. Similar to the case of the square lattice,[4] there are two fixed points of interest. The unstable fixed point occurs at $T=T^*$ and $\gamma=0$, whereas the stable fixed point occurs at $T=0$ and $\gamma=\gamma_0\equiv 1$. We have started at the point $k_BT/J=3.474\,82$ and $\gamma=10^{-4}$, which is near the unstable fixed point and obtained the RG trajectory that leads to the stable fixed point. Such a curve represents the desired surface tension as a function

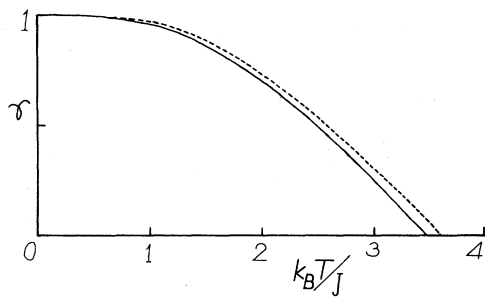

FIG. 3. The result of our real-space RG calculation (solid curve) and a schematic drawing of the exact result (dashed curve) for the surface tension for the Ising model on a triangular lattice.

of the temperature. Figure 3 shows that our curve for γ (in unit of the surface tension at zero temperature) vs T (in unit of J/k_B) agrees surprisingly well with the exact curve[13,14] to within a few percent error only. The method we used to obtain the surface tension curve is essentially the same as that used by Curado *et al.*,[4] but in a more direct approach.

In conclusion, we have calculated the surface tension for the Ising ferromagnet on a triangular lattice using only the lowest-order longitudinal triangular cluster of Chao[9] and obtained excellent results without relying on extrapolation procedures. Thus we show that our longitudinal triangular clusters seem to be very efficient for calculating thermodynamic properties.

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