MONTE CARLO STUDY OF THE PHASE BOUNDARY OF THE ISING ANTIFERROMAGNET

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A conjectured expression for the field dependence of the square Ising antiferromagnet critical temperature is shown to agree with the results of Monte Carlo analysis.

Recently, a technique for computing the interface free energy of the square lattice Ising antiferromagnet was described [1]. The method involved the study of only a restricted class of interface and, on the assumption that the vanishing of this interface free energy corresponds to the critical point $T_c(H)$, the following expression for the boundary separating antiferromagnetic and paramagnetic phases was derived:

$$\cosh[H/T_c(H)] = \sinh[2J_1/T_c(H)] \sinh[2J_2/T_c(H)]. \tag{1}$$

Here $H$ is the applied field, and $J_{1,2}$ the anisotropic nearest neighbor interactions. Eq. (1) reduces to known results in the $H \to 0$ and $T_c(H) \to 0$ limits, and for $H$ small and $J_1 = J_2$ it is consistent with the predictions of high temperature series analysis [2].

In this letter we present the results of a test of the isotropic form of eq. (1), namely

$$\cosh[H/T_c(H)] = \sinh^2[2J/T_c(H)], \tag{2}$$

using the Monte Carlo (MC) method. Since MC techniques only involve systems of finite size, the critical point divergences of the specific heat $C$ and staggered susceptibility $\chi_s$, which occur at $T_c(H)$ in the infinite system, are replaced by finite height peaks whose maxima are shifted away from $T_c(H)$. At $H = 0$ it is known [3] that the location $T_{\text{max}}$ of the specific heat maximum of an $N \times N$ Ising system is given by

$$T_{\text{max}} = T_c(0) + 0.82/N + O(N^{-2}), \tag{3}$$

thus the MC study of a lattice of moderate size (e.g. $N = 60$) should be capable of yielding $T_c$ estimates accurate to within 1%. A result similar to eq. (3) presumably holds also for $H \neq 0$.

We have applied the MC technique [4] to a lattice of size $60 \times 61$ sites with toroidal boundary conditions. Runs of 2400 MC steps per spin (the first 800 steps were not used in the analysis in order to allow convergence) were performed for various values of $H$ and $T$, and a search made for those values of $T$ at which the maxima of $C$ and $\chi_s$ occurred. Once the approximate location of a maximum was found, further runs were made to determine the shape of the peak and thereby provide an estimate of the uncertainty in the value of $T_{\text{max}}$. Each data point used in the final estimation of $T_{\text{max}}$ represents the average of as many

![Graph](image)

Fig. 1. The full curve represents the solution of eq. (2). The horizontal bars indicate the location of $T_{\text{max}}$; for each $H$ the bar on the left corresponds to $C$, the bar on the right to $\chi_s$.  

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as eight separate MC runs using different starting configurations and random number sequences.

The results are summarized in fig. 1. The full curve represents the solution of eq. (2), and the horizontal line segments are the estimates of $T_{c}(H)$ based on the locations of the maxima of $C$ and $\gamma$. In the case of the specific heat it is evident that eq. (2) fits the data remarkably well. The $\gamma$ maxima are seen to occur at consistently higher temperatures than the $C$ maxima; a reasonable explanation is that the finiteness of the lattice affects $\gamma$ more strongly than $C$, and as $N \to \infty$, $T_{\max}(\gamma)$ converges to the limiting value $T_{c}(H)$ at a slower rate than $T_{\max}(C)$. A result analogous to eq. (3) does not exist for $\gamma$ however.

To summarize, on the basis of the MC analysis it would appear that the conjectured form of the phase boundary, eq. (2), is correct. The general anisotropic result in eq. (1) is probably also correct, although it has not as yet been tested.

References