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LETTER TO THE EDITOR

Curie temperature of the square Ising ferromagnet with first-, second- and third-neighbour interactions

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Abstract. The transition temperature for the square-lattice Ising ferromagnet with first-, second- and third-neighbour interactions is calculated by the interface method. The results are apparently fairly accurate, except when the third-neighbour coupling is completely dominating. We check, in particular, a series result for the equivalent-neighbour model to within a few per cent.

The interface method (Müller–Hartmann and Zittarz 1977) yields the exact Curie temperature of many two-dimensional Ising ferromagnets with only nearest-neighbour interactions present (Southern 1978). Among these are the square, triangular and hexagonal lattices. One might ask if this method is a good approximation even when more distant-neighbour interactions are taken into account. Burkhardt (1977) has included the next-nearest-neighbour ferromagnetic interaction on the square lattice, and in this case, the interface method yields an accurate estimate for the Curie temperature. In the limiting cases of only nearest-neighbour and only next-nearest-neighbour interactions the exact Curie temperatures are reproduced, and with both couplings present the interface result probably deviates from the exact temperature by no more than 5%. The most obvious extension of this model is an inclusion of third-neighbour interactions, i.e. a system with the Hamiltonian

$$\mathcal{H} = -J_1 \sum_{1.n} \sigma_i\sigma_j - J_2 \sum_{2.n} \sigma_i\sigma_j - J_3 \sum_{3.n} \sigma_i\sigma_j \tag{1}$$

on the square lattice. The sums run over first-, second- and third-neighbour pairs, respectively, and the interactions are assumed ferromagnetic ($J_n > 0$).

The Curie temperature of this model has not, to my knowledge, been calculated with good precision except in the special case of equivalent neighbours (i.e. $J_1 = J_2 = J_3 = J$). Domb and Dalton (1966) have used series expansion methods to calculate the Curie temperature, T_c, for the equivalent-neighbour model, with the result

$$J/kT_c = 0.1135. \tag{2}$$

If the interface method is capable of giving a transition temperature in good agreement with this result it would be a strong indication that the interface results are accurate approximations even when third-neighbour interactions are taken into account. My calculation is based on a straightforward generalisation of the method developed by Burkhardt in his article. Summing the partition function over interface configurations

on a diagonal interface (see figure 1), the interface free energy per spin along the interface, f_i, is given by

$$\exp(-\beta f_i) = \lambda_m \tag{3}$$

where λ_m is the maximum eigenvalue of the transfer matrix

$$T_{\alpha\gamma} = \exp[-2K_2 - K_1(|2\alpha+1|+|2\gamma+1|) - (2K_2+4K_3)|\alpha+\gamma+1| - 4K_3\delta_{-\alpha,\gamma+1}] \tag{4}$$

$K_n = J_n/kT$, with k the Boltzmann constant and δ the Kronecker delta.

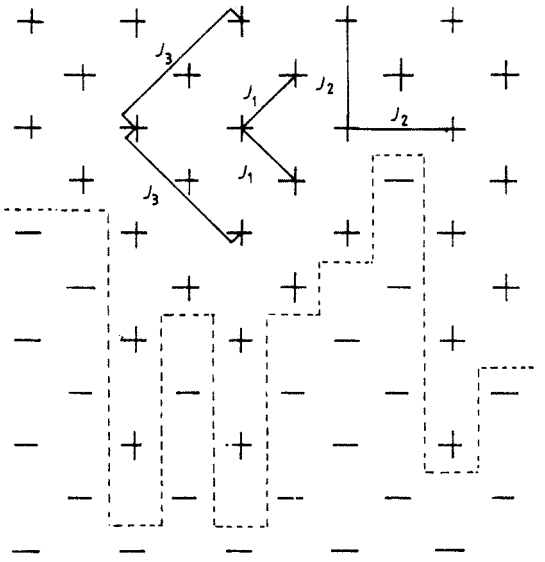

Figure 1. Example of non-overhanging diagonal interface configuration used in the calculation of interface free energy. + and − designate spins of different orientation. J_1, J_2 and J_3 are the three different couplings.

At the critical point the interface free energy vanishes which means that the Curie temperature is determined by $\lambda_m = 1$.

In the limits $J_2, J_3 \to 0$ and $J_1, J_3 \to 0$, respectively, Burkhardt showed that this gives the exact Curie temperature (Onsager 1944)

$$kT_c^1 = 2J_1/[\ln(1+\sqrt{2})] \tag{5}$$

and

$$kT_c^2 = 2J_2/[\ln(1+\sqrt{2})]. \tag{6}$$

In the special case of no nearest-neighbour interactions, $J_1 = 0$, the maximum eigenvalue of T can be evaluated analytically. In this case the relevant eigenvector is x_α = constant. The corresponding eigenvalue is

$$\lambda_m = \sum_{\gamma=-\infty}^{\infty} T_{\alpha\gamma} = \exp(-2K_2)\left(\exp(-4K_3) + \frac{2\exp(-2K_2-4K_3)}{1-\exp(-2K_2-4K_3)}\right) \tag{7}$$

giving the critical condition

$$\exp(2K_2) = \exp(-4K_3) + \sqrt{2}\exp(-2K_3) \tag{8}$$

when J_2 also vanishes, (8) yields the Curie temperature

$$kT_c^3 = 4J_3/[\ln(2+\sqrt{3})] \tag{9}$$

while the exact result is again the Onsager formula (5), about $\frac{2}{3}$ of (9).

I have not been able to evaluate λ_m for arbitrary K_1, K_2 and K_3, but like Burkhardt, I have derived a recurrence relation for the eigenvector x. This can be used for numerical calculation of the Curie temperature for arbitrary interaction strengths. Since $T_{\alpha\gamma} = T_{-(\alpha+1),-(\gamma+1)}$ the relevant eigenvector has the symmetry $x_\alpha = x_{-(\alpha+1)}$, and the eigenvalue equation can be written

$$\lambda_m x_\alpha = \sum_{\gamma=0}^{\infty} (T_{\alpha\gamma} + T_{\alpha,-(\gamma+1)})x_\gamma \tag{10}$$

where α and γ are non-negative integers. Combining (10) and (4) gives the recurrence relation

$$F_0 x_\alpha + F_1 x_{\alpha+1} + F_2 x_{\alpha+2} = 0 \tag{11}$$

with

$$F_0 = 2\exp[-2K_2 - 2K_3 - (6+4\alpha)K_1]\sinh 2K_3 + \lambda_m \exp(-4K_1) \tag{12}$$

$$F_1 = 2\exp[-2K_2 - 4K_3 - (8+4\alpha)K_1][\cosh(2K_2+4K_3) - \exp(-2K_2)] - 2\lambda_m \exp(-2K_1)\cosh(2K_2+4K_3) \tag{13}$$

$$F_2 = 2\exp[-2K_2 - 2K_3 - (10+4\alpha)K_1]\sinh 2K_3 + \lambda_m \tag{14}$$

and the boundary conditions

$$x_0 = \frac{1+\exp(2K_2+4K_3)}{1+2\lambda_m^{-1}\exp(-2K_1-2K_2-2K_3)\sinh 2K_3} \tag{15}$$

$$x_1 = \frac{2\exp(-2K_1+K_2+2K_3)\cosh(3K_2+6K_3) - 2x_0\lambda_m^{-1}\exp(-4K_1-2K_2)\sinh(2K_2+4K_3)}{1+2\lambda_m^{-1}\exp(-6K_1-2K_2-2K_3)\sinh 2K_3} \tag{16}$$

when x is normalised according to the following normalising condition

$$\lambda_m = \exp(-2K_1-4K_2-4K_3)\sum_{\gamma=0}^{\infty}\exp[-(2K_1+2K_2+4K_3)\gamma]x_\gamma. \tag{17}$$

The Curie temperature is found by viewing the normalising condition (17), with the vector x given by (11)–(16), as an equation for the unknown critical temperature when λ_m is put equal to its critical value, $\lambda_m = 1$. This equation is solved numerically.

I have also calculated an expression for the critical condition in the case of weak nearest-neighbour interactions, i.e. an expression valid to the lowest order in K_1. There are two reasons for doing so. First, it is of interest to know how the critical surface approaches the $K_1 = 0$ plane. As will be shown, this plane is a tangent plane of the critical surface. Second, the numerical approach given above is not very useful when $K_1 \leqslant 0.005$. The difference between the right-hand side of (17) and 1 is less than 10^{-10} over large intervals of K_2 and K_3 when $K_1 \leqslant 0.005$. This is probably related to the fact that the right-hand side of (17) equals 1 *identically* when $K_1 = 0$.

In this calculation I found it convenient to introduce the vector $\phi_\alpha = \exp(-2K_1\alpha)x_\alpha$. The elements of this vector are related through a recurrence relation similar to (11). Since the vector x = constant is the relevant eigenvector when $K_1 = 0$, ϕ_α is a slowly varying function of α when K_1 is small. In this limit the recurrence relation can therefore be transformed into a differential equation for $\phi(\alpha) = \phi_\alpha$. Scaling the variable $y = K_1^{1/3}\alpha$ this differential equation can be written

$$\left(-\frac{d^2}{dy^2} + Cy\right)\phi(y) = E\phi(y) \tag{18}$$

with

$$E = CK_1^{-2/3}(K_2^c - K_2) \tag{19}$$

and

$$C = \frac{8}{1+\sqrt{2}\exp(-2K_3)} \tag{20}$$

where the coefficients have been expanded in the small quantities K_1 and $(K_2^c - K_2)$, and higher-order components, giving higher-order contributions to the critical condition, are ignored. K_2^c is the critical value of K_2 when $K_1 = 0$, and is given as a function of K_3 by (8).

The Schrödinger-like differential operator in (18) has a set of pure numbers, E_n, as its eigenvalues. Since the eigenvector associated with the maximum eigenvalue of the matrix T (equation (4)) is positive and symmetric around $-\frac{1}{2}$, we have the boundary conditions $\phi'(0) = 0$ and $\phi(\alpha) > 0$. This gives an unambiguous determination of the eigenvalue $E_0 = E$. The solution of (18) (Morse and Feshbach 1953) gives the critical condition

$$K_1 \approx 2.75038(1+\sqrt{2}\exp(-2K_3))^{-1/2}(K_2^c - K_2)^{3/2}. \tag{21}$$

Thus the critical condition, when K_1 is small, is of the form

$$K_1 = \text{constant}(K_2^c - K_2)^\gamma \tag{22}$$

where the exponent, γ, is independent of K_3. We know that the exact exponent is $\gamma = \frac{7}{4}$ when $K_3 = 0$ (van Leeuwen 1975). My conjecture is therefore that the exact critical condition is of the form (22) with the K_3-independent exponent $\gamma = \frac{7}{4}$.

The critical surface is shown in figure 2. I have used the numerical procedure based on (10)–(16) to evaluate it when $K_1 \geqslant 0.005$, and (21) when $K_1 \leqslant 0.005$. The two parts of the surface join smoothly, there is nowhere more than 2% difference in the two K_1 values along the splicing line.

For the Curie temperature of the equivalent-neighbour model I find

$$J/kT_c = 0.1162. \tag{23}$$

This can be compared with the series expansions value (Domb and Dalton 1966) $J/kT_c = 0.1135$ (equation (2)). The two approximations are clearly in good agreement (within 2.5%). Notice that the interface Curie temperature is slightly *lower* than the series expansion result, as in the case when $K_3 = 0$ (Burkhardt 1977). Since the interface method yields a *higher* Curie temperature than the exact value when the third-neighbour interaction is totally dominant ($J_1/J_3 \approx 0$ and $J_2/J_3 \approx 0$, see equation (9)), this implies that this method is a good approximation even for higher values of

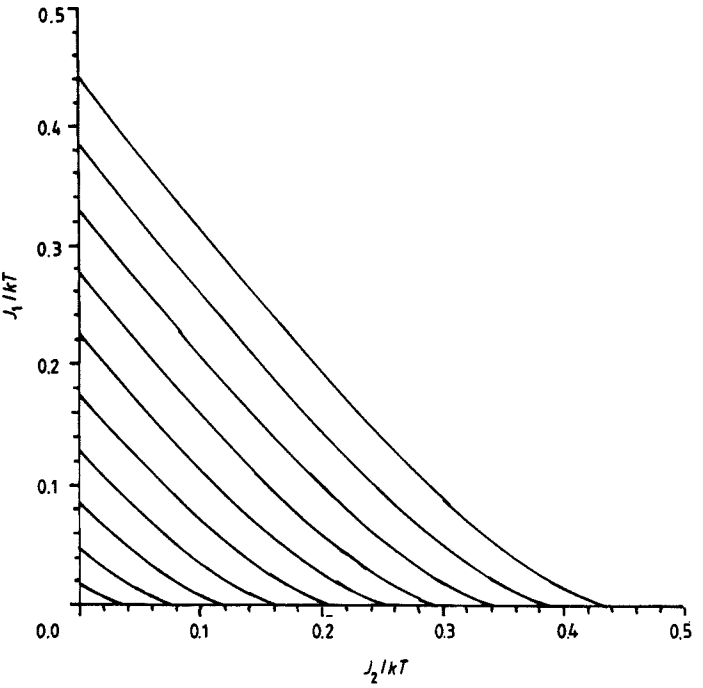

Figure 2. Critical surface. The lines are critical lines for different J_3/kT values, starting from $J_3/kT = 0$ (outer line) with distance $\Delta(J_3/kT) = \frac{1}{40}\ln(2+\sqrt{3}) = \frac{1}{10}K_3^c$. K_3^c is the critical value of J_3/kT when $J_1 = J_2 = 0$.

the ratio $J_3/(J_1+J_2)$ than $\frac{1}{2}$. The conclusion is that the interface method is a good approximation method for determining the Curie temperature of square-lattice Ising ferromagnets, not only with only first- and second-neighbour interactions present, but also when third-neighbour interactions are included. The resulting Curie temperature agrees with the exact value to within a few per cent when third-neighbour interaction is not dominant ($J_3 < J_1 + J_2$). The method only fails seriously when the third-neighbour interaction is totally dominant.

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