The Critical Line of an Ising Antiferromagnet on Square and Honeycomb Lattices

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We show that the singularity of the free energy of Ising models in the absence of a magnetic field on the triangular, square, and honeycomb lattices is related to zeros of the pseudopartition function on an elementary cycle. Using the Griffiths' smoothness postulate, we extend these results to the case in a magnetic field and derive a formula of the critical line of an Ising antiferromagnet, which is in good agreement with the numerical results. [S0031-9007(96)02173-4]

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Since Onsager's famous solution of the square lattice Ising model in the absence of a magnetic field [1], the Ising model became a standard model for testing the scaling and universality hypotheses [2,3]. However, the Ising model in a magnetic field has not been solved exactly so far, although some exact results are known. Of particular interest is to determine the critical line in the (h, T) plane, along which the free energy becomes singular. Yang and Lee [4] proved that for the Ising ferromagnet, the critical line is located at $h = 0$. For the Ising antiferromagnet, the series expansion method was used to obtain related information [5]. Müller-Hartmann and Zittartz obtained the critical line by considering the interfacial tension [6,7]. Wu and coworkers [8,9] formulated the Ising model on the honeycomb lattice as an 8-vertex model and identified the critical line as a locus invariant under a generalized weak-graph transformation. In this paper we introduce a new approach by considering zeros of the partition function on an elementary cycle and using Griffiths' smoothness postulate [10]. A closed-form formula of the critical line of an Ising antiferromagnet is obtained, which is in good agreement with the numerical results [8,11,12].

The partition function of the Ising model in the presence of a magnetic field is given by

$$Z = \sum_{\{S\}} \exp\left[\beta\left(\sum_{\langle ij\rangle} K_{ij} S_i S_j + h \sum_i S_i\right)\right], \tag{1}$$

where $S_i = \pm 1$ and K_{ij} is the interaction strength. The sum over $\langle ij\rangle$ runs over the pairs of nearest neighbors on the lattices. Let us consider the ferromagnetic case, $K_{ij} > 0$. The Ising partition function on an elementary cycle of the triangular, square, and honeycomb lattices (see Fig. 1) can be written, respectively, as

$$z_t = 2[e^{\beta(K_1+K_2+K_3)} + e^{\beta(-K_1-K_2+K_3)} + e^{\beta(-K_2-K_3+K_1)} + e^{\beta(-K_1-K_3+K_2)}], \tag{2}$$

$$z_s = 2[e^{2\beta(K_1+K_2)} + e^{2\beta(K_1-K_2)} + e^{-2\beta(K_1-K_2)} + e^{-2\beta(K_1+K_2)} + 4], \tag{3}$$

$$z_h = 2[e^{2\beta(K_1+K_2+K_3)} + 4e^{2\beta K_1} + 4e^{2\beta K_2} + 4e^{2\beta K_3} + 4e^{-2\beta K_1} + 4e^{-2\beta K_2} + 4e^{-2\beta K_3} + e^{2\beta(K_1+K_2-K_3)} + e^{2\beta(K_2+K_3-K_1)} + e^{2\beta(K_3+K_1-K_2)} + e^{-2\beta(K_1+K_2-K_3)} + e^{-2\beta(K_2+K_3-K_1)} + e^{-2\beta(K_3+K_1-K_2)} + e^{-2\beta(K_1+K_2+K_3)}], \tag{4}$$

where K_j are the interaction strengths. Making the transformation, $p_j = \exp(2\beta K_j) \to p_j' = i p_j$ turns $z(p_j) \to z'(p_j) \equiv z(ip_j)$, which reads as:

$$z_t' = 2i^{3/2}(\zeta_1\zeta_2\zeta_3)^{-1/2}(1 - \zeta_1\zeta_2 - \zeta_2\zeta_3 - \zeta_3\zeta_1), \tag{5}$$

$$z_s' = 2\zeta_1^{-1}\zeta_2^{-1}[(\zeta_1 + \zeta_2)^2 - (1 - \zeta_1\zeta_2)^2], \tag{6}$$

$$z_h' = -2i\zeta_1^{-1}\zeta_2^{-1}\zeta_3^{-1}[(1 - \zeta_1\zeta_2 - \zeta_2\zeta_3 - \zeta_3\zeta_1)^2 - (\zeta_1 + \zeta_2 + \zeta_3 - \zeta_1\zeta_2\zeta_3)^2], \tag{7}$$

where $\zeta_j \equiv \exp(-2\beta K_j)$. One can easily see that the real solutions of $z' = 0$ give the exact relations [3] for the zero-field critical temperatures of an Ising ferromagnet: square: $\zeta_1\zeta_2 + \zeta_1 + \zeta_2 = 1$; triangular: $\zeta_1\zeta_2 + \zeta_2\zeta_3 + \zeta_3\zeta_1 = 1$; honeycomb: $\zeta_1\zeta_2\zeta_3 - \zeta_1\zeta_2 - \zeta_2\zeta_3 - \zeta_3\zeta_1 - \zeta_1 - \zeta_2 - \zeta_3 + 1 = 0$. To state it more clearly,

Lemma 1.—Let the Ising partition function on each elementary cycle of the square, triangular, and honeycomb lattices be $z = z(T, h = 0)$. Make a transformation, $p_j = \exp(2\beta K_j) \to p_j' = i p_j$ and $z(p_j) \to z'(p_j) = z(ip_j)$. Then the critical temperatures are obtained from the real solutions of $z' = 0$.

From this lemma, we deduce, as follows, the results obtained first by Wannier [13]:

(1) For Ising models on square and honeycomb lattices, $z(-K_j) = z(K_j)$, $z'(-K_j) = z'(K_j)$. Thus an

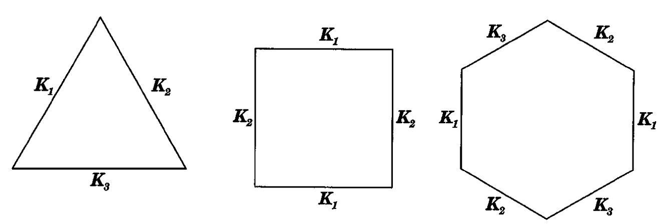

FIG. 1. The elementary cycle of triangular, square, and honeycomb lattices.

antiferromagnetic Ising model with the interaction strength $-K_j$ has the same critical temperature as that of a ferromagnetic Ising model with the interaction strength K_j.

(2) For an Ising antiferromagnet on a triangular lattice, the equation $z_t' = 0$ has no real solution at any finite temperature. Thus, no antiferromagnetic phase transition occurs at any finite temperature.

Now, let us turn our attention to the isotropic case, $K_j \equiv K$. The partition function on an elementary cycle with N sites is exactly that of the one-dimensional Ising model on an N-site chain, with the periodic condition, which is exactly solvable [14]. Thus

$$z = \lambda_+^N + \lambda_-^N, \tag{8}$$

where $\lambda_\pm = e^{\beta K} \pm e^{-\beta K}$. Letting $z = 0$ we obtain

$$e^{2\beta K} = (-i)\cot\frac{(2n+1)\pi}{2N}, (n = 0, 1, 2, ..., N-1). \tag{9}$$

Making the transformation, $p_j \to ip_j$, yields the critical temperatures

$$e^{2\beta K} = -\cot\frac{(2n+1)\pi}{2N}, (n = 0, 1, 2, ..., N-1). \tag{10}$$

Since $K > 0$ we have $e^{2\beta K} > 1$, and thus only $n = N - 1$ is allowed to yield the equation for the *critical temperatures of the isotropic Ising models on triangular, square, and honeycomb lattices*,

$$e^{2\beta K} = \cot\frac{\pi}{2N}, \tag{11}$$

where N is the number of edges of an elementary cycle. On the other hand, Baxter's result [3] is given in the form,

$$e^{-2\beta K} = \tan[\pi(q-2)/4q], \tag{12}$$

where q is the coordination number. Identifying $q = 2N/(N-2)$, we find that Eqs. (11) and (12) are identical.

From Onsager's solution we know that the critical point of the Ising model in the absence of a magnetic field corresponds to the singularity of the free energy [3]. Using lemma 1, we find that *the singularity of the free energy is associated with the zeros of the Ising pseudopartition function on an elementary cycle*.

In 1952 Yang and Lee [4] proposed the celebrated theory of phase transition. By considering the zeros of the grand partition function in the complex fugacity plane, they showed that in the thermodynamic limit the critical point is determined by the positive real roots. When this theory was applied to the ferromagnetic Ising model, they considered zeros of the partition function in the complex magnetic field plane and proved the famous circle theorem. In 1964 Fisher [15] considered zeros of the partition function in the complex temperature plane. He proved that for the Ising model in the absence of a magnetic field and in the thermodynamic limit, the zero distribution approaches the positive real axis and gives the critical point. From lemma 1 we see that for the Ising model on triangular, square, and honeycomb lattices, the positive real roots of the Yang-Lee zeros of the partition function on the infinite lattice in the complex temperature plane are related to the zeros of the partition function on an elementary cycle.

In 1970 Griffiths [10] proposed the smoothness postulate. He reasoned that since on the boundary between the antiferromagnetic and paramagnetic phases there is no *a priori* reason to single out the particular point corresponding to zero field, it is reasonable to assume that the singularity in the free energy does not change its basic character along the boundary. This postulate was verified by Rapaport and Domb [11]. We will use this postulate and take lemma 1 as the boundary condition for $h = 0$. Since at the critical point, $(\partial h/\partial M)_{T_c} = 0$, it follows that along the critical line $(\partial h/\partial M)_T = 0$ [16]. For a square lattice Ising model, the spontaneous magnetization is given by [17]

$$M(T < T_c, h = 0) = \left[1 - \left(\frac{2\zeta_1}{1-\zeta_1^2}\frac{2\zeta_2}{1-\zeta_2^2}\right)^2\right]^{1/8} \sim [z'(T, h = 0)]^{1/8}. \tag{13}$$

According to Griffiths, we assume that in a nonzero magnetic field, near the critical line, the magnetization strength takes the same functional form as the case for $h = 0$,

$$M(T < T_c, h) = g(T, h)[\gamma(T, h)]^{1/8}, \tag{14}$$

where $g(T, h)$ and $\gamma(T, h)$ are nonsingular analytic functions of T and h. $\gamma(T, h)$ is related to the partition function on an elementary cycle, with $\gamma(T, h = 0) = z'(T, h = 0)$. Thus

$$\left(\frac{\partial M}{\partial h}\right)_T = \frac{\partial g}{\partial h}[\gamma(T, h)]^{1/8} + \frac{g}{8}\frac{\partial \gamma}{\partial h}[\gamma(T, h)]^{-7/8}. \tag{15}$$

Since $g(T, h)$, $\gamma(T, h)$, and their derivatives with respect to h do not approach infinity for arbitrary h, along the critical line $(\partial h/\partial M)_T = 0$ requires $\gamma(T, h) = 0$. Therefore ,we might plausibly extend lemma 1 to the case of a nonzero magnetic field. Let the Ising partition function on an elementary cycle of square and honeycomb lattices be $z = z(T, h)$. Make a transformation

$$p_j = e^{2\beta K_j} \to p_j' = ie^{2\beta K_j} \text{ and } |h| \to f(|h|). \tag{16}$$

Thus $z \to z'$ with the boundary condition $f(0) = 0$. Here $f(|h|)$ is assumed to be a real and analytic function of h. *The critical line is given by* $\gamma(T, h) = z' = 0$.

For simplicity let us consider the isotropic Ising model on square and honeycomb lattices. The partition function on an elementary cycle [3] is again given by Eq. (8) with

$$\lambda_\pm = e^{\beta K}[\cosh\beta h \pm (\sinh^2\beta h + e^{-4\beta K})^{1/2}]. \tag{17}$$

Thus $z = 0$ yields

$$\frac{\cosh\beta h}{(\sinh^2\beta h + e^{-4\beta K})^{1/2}} = (-i)\cot\pi\frac{2n+1}{2N}, \quad (n = 0, 1, ..., N-1). \tag{18}$$

Making the transformations, we obtain the critical line,

$$e^{-4\beta K} = \tan^2 \pi \frac{2n+1}{2N} \cosh^2 \beta f(|h|) + \sinh^2 \beta f(|h|),$$
$$(n = 0, 1, ..., N-1). \quad (19)$$

It is interesting to note that for an Ising ferromagnet ($K > 0$), if $h \neq 0$ and $T < T_c$, Eq. (19) has no real solution and no phase transition occurs, which is consistent with the conclusion of the Yang-Lee circle theorem [4].

For an Ising antiferromagnet $K < 0$, the critical line is obtained as

$$e^{4\beta|K|} = e^{4\beta_c|K|} \cosh^2 \beta f(|h|) + \sinh^2 \beta f(|h|). \quad (20)$$

$f(|h|)$ can be expanded as

$$f(|h|) = A|h| + B|h|^2 + \cdots. \quad (21)$$

Consider the limiting case $T \to 0$. Taking the logarithm of Eq. (20), we obtain

$$|f(|h|)| = 2|K| - \frac{1}{2} kT \ln \frac{1 + e^{4\beta_c|K|}}{4}. \quad (22)$$

Thus $|f(|h_0|)| = 2|K|$ with $h_0 = h(T=0)$. Consider another limiting case $\beta \to \beta_c^+$. Substituting Eq. (21) into Eq. (20) and keeping only the lowest order terms, we obtain the well-known scaling law [11],

$$\frac{T_c - T}{T_c} = \frac{1 + e^{-4\beta_c|K|}}{4} \frac{A^2}{|K|kT_c} |h|^2. \quad (23)$$

Using the exact result [11,12] $|h_0| = q|K|$ and Eq. (12), to the first-order approximation of $f(|h|)$, we have $A = 2/q$. Thus the critical line is given by

$$e^{4\beta|K|} = \cot^2\left[\frac{\pi(q-2)}{4q}\right] \cosh^2\left(\frac{2\beta h}{q}\right) + \sinh^2\left(\frac{2\beta h}{q}\right). \quad (24)$$

It is interesting to note that Eq. (24) contains only h, T, K, and q.

For the square lattice ($q = 4$), using Eqs. (22) and (23) we obtain, in the limit $T \to 0$, $|h| = 4|K| - 0.534800kT$ and as $T \to T_c^-$, $(T_c - T)/T_c = 0.03227(h/K)^2$. The numerically obtained formuli are $-\beta|K| = -\beta h/4 - 0.166752(3)$ as $T \to 0$ [12,18] and $(T_c - T)/T_c = 0.0380(h/K)^2$ as $T \to T_c^-$ [11]. Using these numerical results, we improve our results to the third order, obtaining $f(|h|) \approx 0.542578|h| + 0.0034873|h|^2/|K| - 0.00353295|h|^3/|K|^2$. The critical line is shown in Fig. 2(a). We compare our results with the Müller-Hartmann and Zittartz's formula [6] and the Wu and coworkers' formula [9], which are good approximations. At some discrete points the data generated from these formuli are also plotted in the figure. Our critical line encompasses the other two, but very close to that of [9]. We see that the agreements are good.

For the honeycomb lattice ($q = 3$), in the limit $T \to 0$, we get $|h| = 3|K| - 0.9877kT$, and as $T \to T_c^-$, $(T_c - T)/T_c = 0.07841(h/K)^2$. The numerically obtained formula is $|h| = 3|K| - 1.030366kT$ as $T \to 0$ [8]. Using the numerical results given in [8], we have a third order approximation, $f(|h|) \approx 0.69151507|h| - 0.003105195|h|^2/|K| - 0.001725869|h|^3/|K|^2$. It is plotted in Fig. 2(b). The data given in [8] are marked as a cross. The agreements are good.

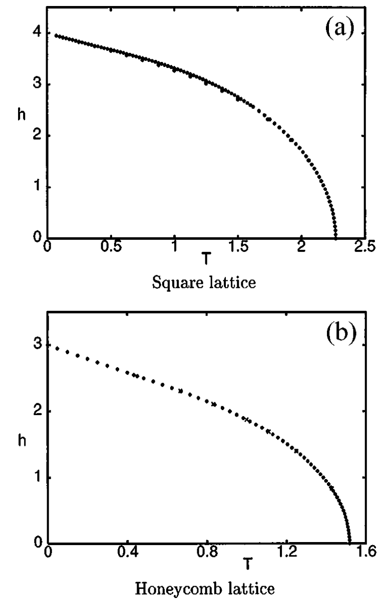

FIG. 2. The critical line of the Ising antiferromagnet. h is in units of $|K|$ and T is in units of $|K|/k$.

If we include more higher order terms in the approximation, we will obtain better results. For the anisotropic cases, we can use the same procedure to obtain the critical line. The shape of the critical line remains unchanged. Details will be published elsewhere.

In conclusion, we have shown that the singularity of the free energy of the Ising model in the absence of a magnetic field on triangular, square, and honeycomb lattices is associated with the zeros of the pseudopartition function on an elementary cycle. Using the Griffiths' postulate, we extended these results to the case with a nonzero magnetic field and obtained the critical line of the Ising antiferromagnet on square and honeycomb lattices. Our theoretical results are in good agreement with the numerical ones.

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